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Modelling and simulation of InAs quantum dots grown on GaAs substrate for optical performances enhancing.

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Abstract— **The objective of this work falls within the framework of general efforts to achieve an optimal growth of a double heterostructure made of the two semiconducting materials InAs and GaAs. Particularly, we are interested in the impact of the growth control parameters on the physical properties of the two-dimensional InAs mono-layer. We report here a complete but not exhaustive analysis of the electronic states of an InAs based quantum dots layers growth on a GaAs substrate. Both modelling and simulation were performed in this work in order to achieve our calculations on the two existing geometries (rectangular and elliptical) of InAs quantum dots. This study has allowed us to draw two graphics. The first one provides the change of the electronic transition energy as a function of quantum dots' radius whilst the second one concerns the absorption coefficient as a function of the incident photon wavelength. The curves we have obtained indicate clearly that the geometrical shape of the InAs quantum dot does significantly alter the above different parameters. We could therefore confirm that the more appropriate geometry is the elliptical one because of the higher performances.**

***Keywords*— Quantum dots, InAs/GaAs, transition energy, absorption coefficient, simulation/modelling**

I. INTRODUCTION

Reducing dimensionality has shown to provide new nanometric compounds with possible semiconductors applications. During the last years, the process to provide such materials has been fruitful and it is possible at the present time to produce quantum dots of good quality and well defined shape. It is indeed rational or even indispensable to study their properties in the view to further optimize the synthesis parameters. The implementation of these materials in existing optoelectronic devices or developing new applications is also envisaged [1].

Previous reports have pointed out the importance of quantum dots in the field of optoelectronics. It is worth to recall here for example that the quantum density in In(Ga)As/GaAs system reaches a values around $1010/cm^2$. Such values have been showed to deteriorate the capacities of the system as it causes the gain saturation [2]. Our study constitutes a contribution to the understanding for the optimization of the synthesis/structural properties/optical properties chain of quantum dots. The choice of the InAs/GaAs structure arises from the great deal of interest that attracts this system for the specific properties it offers. Unique plan (mono-layer) of InAs growth on GaAs is widely studied and represent nowadays a typical reference in the domain and further investigations are believed to provide clues for other systems. We suggest in this report a numerical study of structures made from Indium and Gallium elements. The structural study of the above listed materials should provide the knowledge of their optical properties. We argue then that this work may be considered as a part of the efforts made in the field of micro-electronics research domain as it is based on the control and the analysis at nanometric scale.

II. THEORY

In order to enhance our understanding of physical phenomena that may occur in a quantum dots, it is necessary to know their internal structure. It is then indispensable to elaborate models as close as possible to reality helpful for the determination of the observable optical transitions. Indeed, there is no electronic band structure for three-dimensional confinement materials. Only discrete energy levels are possible for these materials because of the discrete energy state. Previous calculations has shown that in spite of the diversity of results obtained within different models only quantum dots with size larger than 10 nm have many confined electronic states and the latter participate necessary in the excited states [3,4]. Strong selection rules then would exist for the electron-hole recombination in the here studied InAs/GaAs quantum dots [5].

- The transition energy used in this work is given by:

$$E_{tr} = E_g + E_e + E_h \quad (1)$$

where:

E_e is the electron quantification energy.
E_h is the hole quantification energy.
E_g is the band gap energy.

- The absorption coefficient $\alpha(E)$, for a photon energy E higher than the band gap energy E_g, is given by the following equation [6]:

$$\alpha(E) = \alpha_0 . (E-E_g)^{1/2} . E^{-1} \quad (2)$$

where: α_0 is a constant and E_g is the band gap energy.

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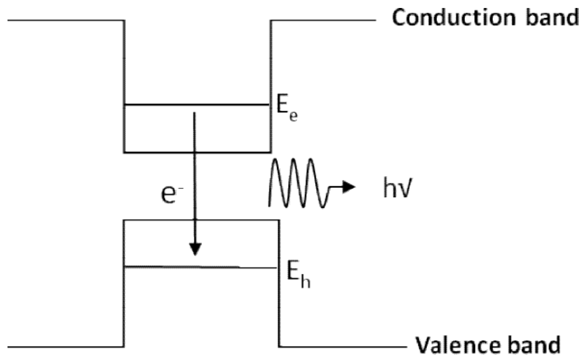

Fig. 1 Principle scheme of the band structure illustration for self-organised quantum dots.

III. Results And Discussion

We have first realized calculations of the electronic transition energy as a function of quantum dots radius for each geometrical type (elliptic and rectangular). We have then performed simulations for radius length varying between 30 and 100 Å. The results are summarized in the figures (2) and (3).

Figure (2) shows the results for the elliptical geometry. We can see that the curves of the electronic energy transitions from v1 level to c1 level (noted Nv1-c1) and from v2 level to c1 level (noted Nv2-c1) both decrease as the quantum dots radius increases. We note however that the first curve shows systematically lower value than the second for a given quantum dots radius value.

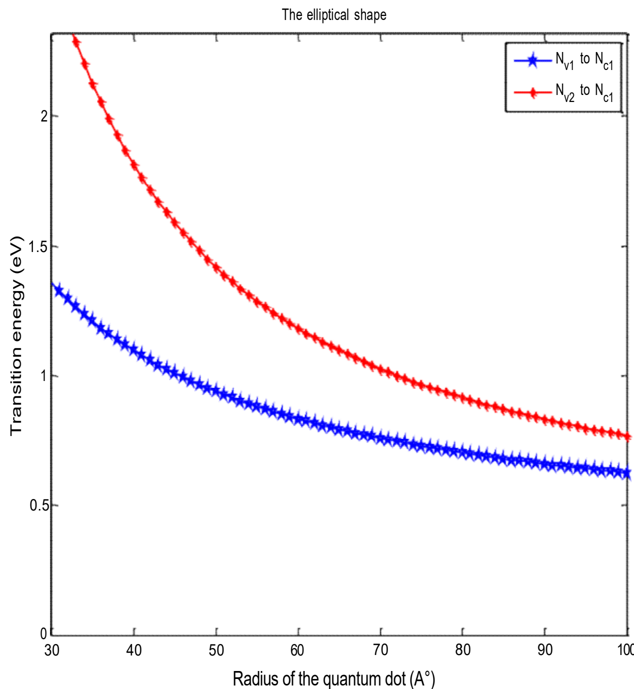

Fig. 2 Electronic transition energy as a function of the radius of elliptical InAs quantum dots grown on GaAs substrate

Figure (3) shows the results for the rectangular geometry. We can see the same behaviour like seen for the elliptical geometry case as the curves of the electronic energy transitions from v1 level to c1 level (noted Nv1-c1) and from v2 level to c1 level (noted Nv2-c1) decreases again as the quantum dots radius increases. We note also that the first curve shows systematically lower value than the second for a given quantum dots radius value.

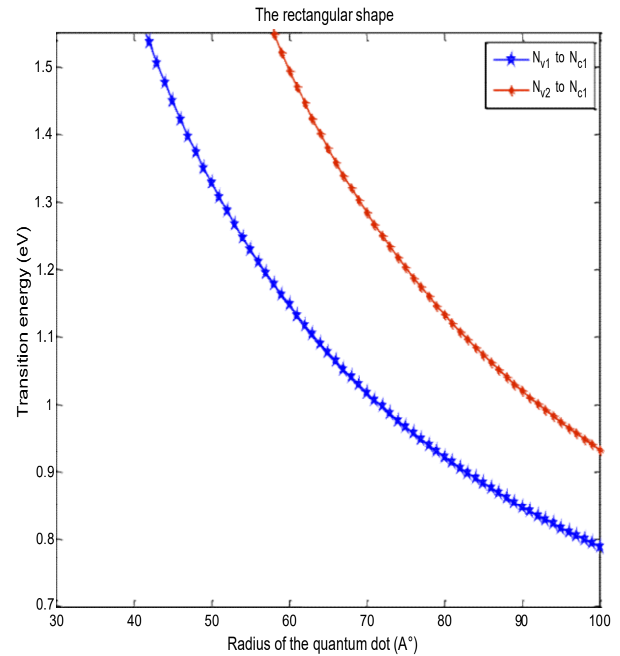

Fig. 3 Electronic transition energy as a function of the radius of rectangular InAs quantum dots grown on GaAs substrate

The energy levels are listed for different values of quantum dots radius in the following table:

TABLE I

	Radius (Å)		35	45	55	65	75	85	95
Energy (eV)	Elliptic	N_{v1_c1}	1.21	1.00	0.88	0.79	0.72	0.68	0.64
		N_{v2_c1}	2.12	1.59	1.28	1.09	0.96	0.87	0.79
	Rectangular	N_{v1_c1}	1.97	1.44	1.22	1.07	0.96	0.88	0.81
		N_{v2_c1}	2.71	2.03	1.63	1.38	1.20	1.07	0.97

In summarize for the first part, these figures enable us to observe a shift of the inter-levels transition energy when the quantum dots are larger. Thus the analysis of the above patterns shows that the transition energies highly depend on the size of the quantum dot. In fact, these energies are inversely proportional to the quantum dots size. The observed decrease is known to be caused by the variation of confinement energy [7,8]. Furthermore, the difference energy between the spectral lines decreases when the quantum dots diameter increases. These observations confirm the quantum confinement effect expected for this structure as the variation of the radius, i.e. volume, of the quantum dots enable then to

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modify their electronic and corollary should affect the optical properties. The transition energy for the elliptic case presents an important change as compared to the rectangular one.

The second part of this work concerns the simulation of the absorption coefficient as a function of the incident photon wavelength. We have considered the two geometries seen for the InAs quantum dots of size of 50 Å. The results are summarized in figures 4 and 5.

Figure (4) shows the results for the elliptical geometry. We can see that the curve of the absorption coefficient present a broad peak between 370 nm and 680 nm. The absorption coefficient reaches a maximum value of $15{,}20.10^5$ μm^{-1} around 490 nm.

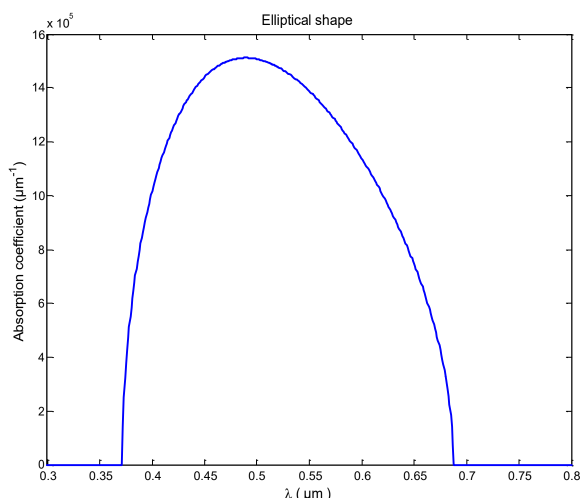

Fig. 4 Absorption coefficient α as a function of the incident photon wavelength λ for elliptical InAs quantum dots grown on GaAs substrate.

Figure (5) shows the results for the rectangular geometry. We can see that the curve of the absorption coefficient presents a broad peak between 430 nm and 550 nm. The absorption coefficient reaches in this case a maximum value of $5{,}93.10^5$ μm^{-1} around 490 nm.

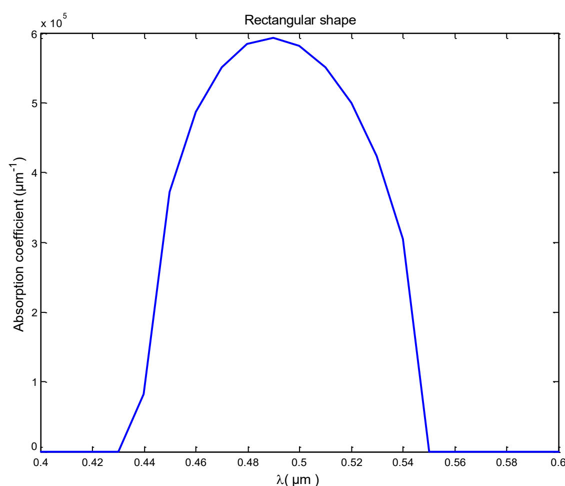

Fig. 5 Absorption coefficient α as a function of the incident photon wavelength λ for rectangular InAs quantum dots grown on GaAs substrate.

We can clearly state on the fact that the absorption profile for the elliptic geometry presents an important broadening than for the case of rectangular geometry. Furthermore, the comparison between the two curves enables to exhibit a much higher difference in intensity. The elliptic case presents an intensity three times higher than for the rectangular one.

The above analysis show clearly that the absorbance of the sample with the elliptical geometry is higher which provides again another advantage to the use of this InAs quantum dots to obtain higher performances.

The intensity of the absorption band and absorbance may explain quantitatively. It is shown elsewhere that they are to be a function of the structure as well as the number of the particles which absorb the incoming beam radiation [9]. We have not carried a quantitative study here.

IV. Conclusions

The present structural/optical properties study of the InAs quantum dots grown on GaAs substrate have revealed many differences when different geometric properties are considered. We could in fact observe a shift of the electronic energy transition and absorption coefficient to higher energies. These parameters are indeed important for the determination of the number of absorbed photons and therefore the produced carriers [10]. This change is thought to be caused the confinement energy when the size of the particles is reduced as well as when the geometry is changed from elliptical to rectangular and vice versa.

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