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Influence of graded interfaces on the exciton energy of type-I and type-II Si/Si_{1-x} Ge_x quantum wires

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Abstract The exciton properties of $Si/Si_{1-x}Ge_x$ cylindrical quantum wires (QWRs) are calculated using the variational method and taking into account the existence of an interface layer between the materials. We consider two possibilities for the conduction band lineup, type-I and type-II. Our numerical results show that an interfacial fluctuation of 15Å in a $Si_{0.85}Ge_{0.15}$ ($Si_{0.70}Ge_{0.30}$) type-I (type-II) wire of 50Å wire radius leads to an exciton energy blue shift of the order of 10 (10) meV.

Introduction

With the success of low dimension semiconductor structures, like quantum wells (quasi-bi-dimensional system) and quantum dots (zero-dimensional systems), relevant theoretical and experimental interest in studying one dimensional semiconductor systems have been presented. Advances in growth materials techniques made possible to confine charge carriers in quite thin wires, named quantum wires (QWRs). These structures in which electrons and holes are bi-dimensionally confined, having only one free dimension, have been successfully used in opto-electronics and biological sensors, where strong confinement is required [1, 2, 3, 4].

Banyai et al [5] studied excitons in type-I QWRs using a variational approach and assuming infinite potential barriers. They found that the exciton binding energy is vastly increased in these structures when compared to three-dimensional (3D) and bi-dimensional (2D) cases. Later, J. M. Rorison [6] studied excitons in *GaAs/AlAs* QWRs, and concluded that the exciton binding energy in type-II wires is substantially larger than that energy of type-II quantum well systems. Since this heterostructure forms a type-II system only for thin wires, where the energies are naturally larger, he also showed that the binding energies of these type-II wires are greater than those ones for type-I systems, for the appropriate wire sizes. More recently, comparisons between experimental measurements of PL peak energies and theoretical results obtained within the effective mass approximation were made by Y. Sidor et al [7] and J. Maes et al [8] for *InAs/InP* QWRs, where a good agreement was attained.

The alloy SiGe allows the construction of heterojunctions that may be directly integrated with Si circuits already existent, giving improvement in the capacity of silicon technology compatible systems [9]. Much experimental data of these materials is available. Although there is consensus that the heterostructure creates a well potential for holes in the valence band, there is still a controversy about the conduction band alignment. It has been reported that the conduction band might form a well (type-I) or a barrier (type-II) for electrons depending on the germanium concentration in the alloy [10].

In this work we use a one parameter variational method to calculate exciton energies in cylindrical semiconductor quantum wires with type-I (type-II) band alignment, where the charge carriers are spatially confined in the same (different) materials. In our system, we take into account the existence of graded

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interfaces between materials. We propose a Hamiltonian that describes the carrier confinement, considering an effective mass depending on the spatial coordinates [11] and evaluate the exciton energy varying the wire radius and interface thickness, for a cylindrical $Si_{1-x}Ge_x$ wire surrounded by a Si layer. The material parameters of the alloy were obtained by interpolation of pure Si and Ge parameters.

Theoretical model

Due to the symmetry of our problem, we will use circular cylindrical coordinates ρ,θ,z. Considering only the ground state, which is θ-independent (m = 0), if we takeρ as the confinement direction and z as the free direction, the Hamiltonian that describes our system can be written as

$$H_{exc} = -\frac{\hbar^2}{2}\left[\frac{1}{\rho_i}\frac{\partial}{\partial\rho_i}\left(\frac{\rho_i}{m_i^{\parallel}(\rho_i)}\frac{\partial}{\partial\rho_i}\right)\right] + V_i(\rho_i) - \frac{\hbar^2}{2\mu^{\perp}}\frac{\partial^2}{\partial z^2} - \frac{e^2}{4\pi\varepsilon\sqrt{\left|\overrightarrow{\rho_e} - \overrightarrow{\rho_h}\right|^2 + z^2}}, \quad (1)$$

where (i = e,h), $m_i^{\parallel}$ is the in plane ρ-dependent effective mass of each charge carrier, $\mu^{\perp}$ is the electron-hole reduced mass in z-direction, and $z = |z_e - z_h|$.

To take into account the existence of a graded interface between materials, we consider the Ge composition χ of the alloy as ρ-dependent, similar to the model of Freire et al [12]. For a $\chi(\rho_i)$ decreasing linearly at the interfacial region, we have

$$\chi(\rho) = \begin{cases} x, & 0 \le \rho \le \rho_1, \\ x - (\rho - \rho_1)x/W, & \rho_1 < \rho \leqslant \rho_2, \\ 0, & \rho > \rho_2, \end{cases} \quad (2)$$

where ρ_1 and ρ_2 are the limits of the interfacial region and $w = \rho_2 - \rho_1$ is the interface thickness.

Thus, $V_i(\rho_i)$ and $m_i^{\parallel}(\rho_i)$ are expressed as function of $\chi(\rho_i)$ following $V_i(\rho_i) = Q_i[e_1\ \chi(\rho_i) + e_2\ \chi^2(\rho_i)]$ and $m_i^{\parallel}(\rho_i) = \{m_{i,Ge}\chi\ (\rho_i) + m_{i,Si}\ [1-\chi(\rho_i)]\}$, where e_1 and e_2 are interpolation parameters found in literature and Q_i is the band offset [10].

Using a variational approach, we assume a trial wave function of the form

$$\Psi(\rho_e, \rho_h, z) = \psi_e(\rho_e)\psi_h(\rho_h)\phi(z), \quad (3)$$

where $\psi_{e(h)}$ is the wave function of the confined electron (hole) and $\varphi(z)$ is chosen to be a gaussian-type ''orbital'' function [13]

$$\phi(z) = \frac{1}{\eta}\left(\frac{2}{\pi}\right)^{1/4}\exp\left(-\frac{z^2}{\eta^2}\right), \quad (4)$$

with η as the variational parameter that minimizes the exciton binding energy.

For type-I systems, we use this trial function and, for each carrier, we obtain a Schrödinger-like equation

$$-\frac{\hbar^2}{2}\left[\frac{1}{\rho_i}\frac{\partial}{\partial\rho_i}\left(\frac{\rho_i}{m_i^{\parallel}(\rho_i)}\frac{\partial}{\partial\rho_i}\right)\right]\psi_i(\rho_i) + V_i(\rho_i)\psi_i(\rho_i) = E_i\psi_i(\rho_i), \quad (5)$$

solved by a discretization method [14] to find the eigenvalues and wave functions. After this, we are able to calculate $E_x = E_e + E_h - |E_b|$, where the binding energy E_b is given by

$$E_b = \frac{\hbar^2}{2\mu^{\perp}\eta^2} - \frac{1}{\eta}\frac{e^2}{4\pi\varepsilon}\sqrt{\frac{2}{\pi}}\int_{V_\Omega}\frac{|\psi_e(\rho_e)|^2|\psi_h(\rho_h)|^2\exp(-2z^2/\eta^2)}{\sqrt{\rho_e^2 + \rho_h^2 - 2\rho_e\rho_h\cos(\theta) + z^2}}dV_\Omega. \quad (6)$$

In the last (Coulomb) term, the integration must be carried out over a cylinder which has an infinite interval along the z direction, and $dV_\Omega = \rho_e\ d\rho_e\ \rho_h\ d\rho_h\ d\theta$.

We may simplify the integral over the cylinder, and then the binding energy takes the form [15]

$$E_b = \frac{\hbar^2}{2\mu^{\perp}\eta^2} - \frac{e^2}{2\varepsilon\eta}\sqrt{\frac{2}{\pi}}\int_0^{2\pi}\int_0^{+\infty}\int_0^{+\infty}|\psi_e(\rho_e)|^2|\psi_h(\rho_h)|^2\exp(a)K_0(a/2)\rho_e\rho_h d\rho_e d\rho_h d\theta \quad (7)$$

where $a = -2\left|\overrightarrow{\rho_e} - \overrightarrow{\rho_h}\right|/\eta$ and K_0 is the modified zeroth-order Bessel function of second kind. We are using the electron-hole relative angular coordinate $\theta = \theta_e - \theta_h$. Since we are considering only the ground state, the wave functions have no angular dependence, *i.e.* $m = 0$. We may perform numerically these integrals and then obtain the exciton emission energy of the system, given by $E_{exc} = E_x + E_{gap}$.

With a type-II band alignment, our problem becomes considerably different. Now, the potential for the electron has a step form, which implies that the electron is no more confined due to the bands mismatch of the materials of the wire, but it is just bound by the Coulomb interaction. Thus, if one tries to solve the Schrödinger equation with the one-particle Hamiltonian for the electron, it must lead to the electron an energy $E_e = 0$. In this way, to solve the

type-II problem we use the form of Ψ given by Eq. (3) in $H_{exc}\,\Psi = E_x\,\Psi$, multiply by the complex conjugate of the ρ_h and z dependent parts of Eq. (3) and then integrate on these coordinates [16]. This procedure leads to the following differential equation for $\psi_e\,(\rho_e)$

$$\left[-\frac{\hbar^2}{2\rho_e}\frac{\partial}{\partial\rho_e}\left(\frac{\rho_e}{m_e^{\parallel}(\rho_e)}\frac{\partial}{\partial\rho_e}\right)+V_e(\rho_e)+E_h+\frac{\hbar^2}{2\mu^{\perp}\eta^2}-I(\eta,\rho_e)\right]\psi_e(\rho_e)=E_x\psi_e(\rho_e), \tag{8}$$

where the effective (Coulomb) attractive potential is given by

$$I(\eta,\rho_e)=\frac{e^2}{4\pi\varepsilon\eta}\sqrt{\frac{2}{\pi}}\int_0^{2\pi}\int_0^{+\infty}|\psi_h(\rho_h)|^2\exp(a)K_0(a/2)\rho_h d\rho_h d\theta \tag{9}$$

In Eq. (8), the parameter η is determined by minimizing the fundamental exciton energy E_x, just like in the variational method developed for type-I wires, and now the exciton binding energy is evaluated by $E_b = E_h - E_x$.

Results

We calculated the recombination energies and exciton total energies of $Si/Si_{1-x}Ge_x$ QWRs for several wire radii and interface thicknesses, with x = 0.15 (type-I band alignment) and x = 0.30 (type-II band alignment) QWRs. The parameters related are listed in Table 1.

The effective potential for electrons and holes in a type-I (type-II) system is shown in Fig.1a, b, where can be clearly seen a depression in the type-II electron potential, caused by the electron-hole coulomb interaction in the heterostructure potential, which is responsible for the electron bound state. The dotted lines are the respective wave functions for these potentials.

In Fig. 2 we show the electron-heavy hole recombination energy of type-I (a) and type-II (b) QWR as a function of the wire radius, respectively in $Si/Si_{0.85}Ge_{0.15}$ and $Si/Si_{0.70}Ge_{0.30}$ wires, with interface thickness

Table 1 Selected properties of Si and Ge, which are used to obtain values for $Si_{1-x}Ge_x$ by interpolation [8]

	a(Å)	E_g(eV)	$\varepsilon(\varepsilon_0)$	$m_e(m_0)$	$m_{hh}^{\perp}\,(m_0)$	$m_{hh}^{\parallel}$
Si	5.43	1.12	12.1	0.191	0.277	0.216
Ge	5.65	0.66	16.0	0.081	0.208	0.057

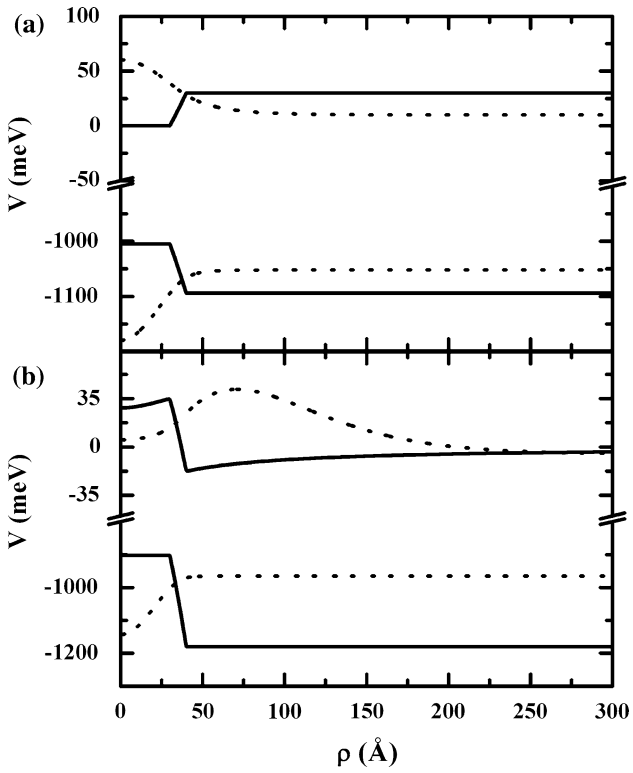

Fig. 1 (**a**) Heterostructure potential (solid) for electrons and holes and their respective wave functions (dotted) as functions of ρ, in a 40Å radius type-I QWR, considering a 10Å interface thickness. (**b**) The same, but for a type-II QWR, where we may observe a depression on the electron potential near the region of the interface between materials

w of 0Å (solid), 5Å (dashed), 10Å (dotted) and 15Å (dashed-dotted). The respective total exciton energies are shown in Table 2 and Table 3.

In type-I and type-II cases, for wire radii smaller than 100Å there is a blueshift of the recombination energy when the existence of graded interfaces is taken into account. The energies of type-II wires are lower than those energies for type-I, which is expected, since in type-II systems the electron and the hole are localized in different materials.

For a 50Å radius $Si/Si_{0.85}Ge_{0.15}$ QWR with interface thickness w = 15Å, the increase on the total exciton energy is about 10 meV in relation to the abrupt case. Moreover, considering this interface thickness, there is an average increase on the binding energies about 5.5%. The results also show total exciton energies in a range from 1.015 eV up to 1.115 eV and recombination energies varying from 1.027 eV up to 1.129 meV.

The total exciton energies in type-II QWR are found with values varying from ~0.908 eV up to ~1.016 eV and the binding energies are of order of 4.5 meV. For a $Si/Si_{0.70}Ge_{0.30}$ with 40Å wire radius, the increases in the exciton total and recombination energies, when one

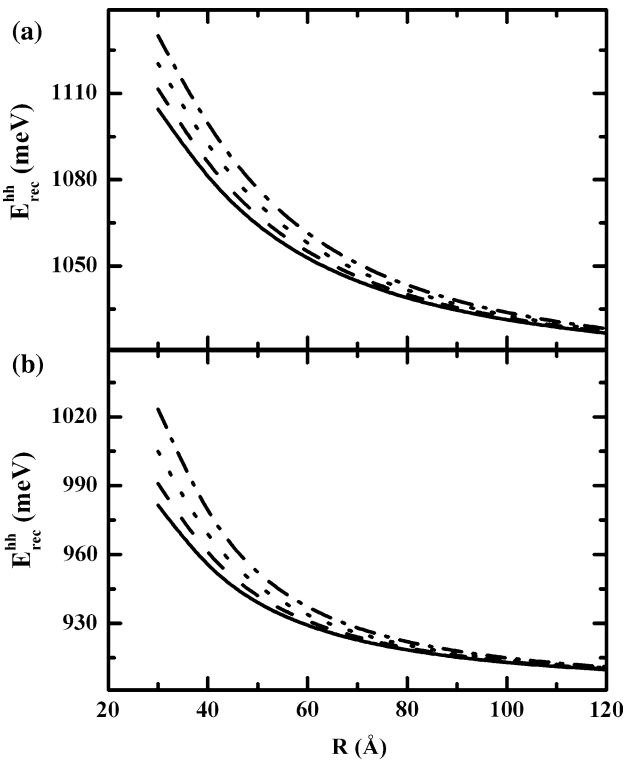

Fig. 2 Electron-heavy hole recombination energies in type-I $Si/Si_{0.85}Ge_{0.15}$ (**a**) and type-II $Si/Si_{0.70}Ge_{0.30}$ (**b**) QWR, considering interface thickness w of 0 Å (solid), 5 Å (dashed), 10 Å (dotted) and 15 Å (dashed-dotted). The interface layer considered comes from the wire thickness

Table 2 Exciton energies for $Si/Si_{0.85}Ge_{0.15}$ type-I QWR, considering several values of wire radius and interface thickness

R\ w	0 Å	5 Å	10 Å	15 Å
30 Å	1084.04	1091.97	1102.44	1114.56
50 Å	1043.35	1046.23	1050.08	1054.76
70 Å	1027.21	1028.45	1030.12	1032.14
90 Å	1019.62	1020.25	1021.11	1022.08
110 Å	1015.67	1015.99	1016.45	1016.97

Table 3 Exciton energies for $Si/Si_{0.70}Ge_{0.30}$ type-II QWR, considering several values of wire radius and interface thichness

R\ w	0 Å	5 Å	10 Å	15 Å
30 Å	975.683	984.798	998.561	1016.66
50 Å	933.949	936.714	940.785	946.061
70 Å	919.105	920.259	921.922	924.011
90 Å	912.290	912.870	913.695	914.711
110 Å	908.648	908.977	909.440	910.005

considers a $w = 15$Å interface thickness, are about 20 meV and 22 meV respectively, if one compares to the abrupt case.

Conclusion

We have performed a theoretical study on the exciton recombination and total energies of semiconductor capped quantum wires with type-I and type-II band alignment. In the later case, where the electrons and holes are in different regions of space, the energies are lower than in the former case, where the carriers are in the same material. Our numerical results show that interface fluctuations of only 15Å in a $Si/Si_{0.85(0.70)}Ge_{0.15(0.30)}$ type-I (type-II) QWR with 50Å wire radius leads to a 10 meV blueshift on the *e-hh* exciton energies. The results of this work allow us to assure that, for an improved description of the exciton energy in $Si/Si_{1-x}Ge_x$ QWRs the existence of graded interfaces must be taken into account, particularly for thin wires.

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