Electron-Phonon Scattering in Graded Quantum Dots

G. S. Diniz, Fanyao Qu, O. O. Diniz Neto, and A. M. Alcalde
Instituto de Física, Universidade Federal de Uberlândia,
Caixa Postal 593, 38400-902, Uberlândia-MG, Brazil

Received on 4 April, 2005

Theoretical calculations of electron-phonon scattering rates in GaAs/$Al_xGa_{1-x}As$ spherical quantum dots have been performed by means of effective mass approximation in the frame of finite element method. The influence of a roughness interface and external magnetic fields are analysed for different scattering rate transition. Our results open interesting channels for electron dephasing times manipulation.

Keywords: Theoretical calculations; Electron-phonon scattering; GaAs/$Al_xGa_{1-x}As$

I. INTRODUCTION

One of the most common procedures of fabricating semiconductor low-dimensional structures is by epitaxial growing of compositionally graded alloys as $Al_xGa_{1-x}As$. Thus, structures that confine electrons are made by changing the aluminum x fraction during crystal growth leading to a compositional graded alloy. The resulting band structure variation produces a spatially varying conduction band minimum. Hence, an electron added to the conduction band through doping, optical excitation or electrical injection, "sees" a position-dependent potential. By varying the concentration appropriately, one can engineer confining potentials that restrict electron motion in a particular spatial direction. Intentional grading can be used to control the strain in quantum dot structures [1], reduce the electron capture times [2] or modify the electron-phonon scattering [3,8].

In this work, theoretical calculations of electron-phonon scattering rates in GaAs/$Al_xGa_{1-x}As$ spherical quantum dots (SQD's) have been performed by means of an effective mass approximation in the frame of the finite element method (FEM)[4]. The influence of a symmetry breaking of the wave function on the electron dephasing times due to the electron-phonon interaction is investigated for various SQD sizes and grading profiles. It is demonstrated that the electron-acoustic phonon scattering rates strongly depends upon both SQD size and magnetic field strength. For different allowed transitions, given by the selection rules Δm= 0 and Δm= 1, where m is the magnetic quantum number of the conduction electron states, the scattering rates present opposite magnetic field dependent behaviour, which can be tuned by a properly choice of magnetic field strength and compositional grading.

II. THEORY AND RESULTS

The Hamiltonian for a single conduction electron in presence of magnetic field **B** = (0,0,B), with a vector potential **A** = (-y, x,0)B/2, is $H = H_0 + H_B + V$, where H_0 includes the kinetic energy. The term H_B is given by -$eBmh/2m* + e^2B^2(x^2+y^2)/8m*$, with m =0, ±1, ±2..., and m* is the electron effective mass. The confinement graded potential V [5] is described by the following equations (in eV units):

$$V(\rho) = \begin{cases} 0 & \rho \le R-\xi, \\ 0.6(1.155y+0.37y^2) & R-\xi < \rho \le R+\xi, \\ 0.6(1.155x+0.37x^2) & \rho > R+\xi, \end{cases}$$

where R represents the quantum dot radius, ξ the interface thickness, x is the aluminum concentration (in this work, $x = 0.3$) and $y = x(\rho+\xi$ -$R)/R$, representing the linear molar fraction in the interface region.

The electron effective mass is described by $m*/m_e$ =0.067 for GaAs, $m*/m_e$ =0.067+0.083y for the interface region, $m*/m_e$ =0.067+0.083x for $Al_xGa_{1-x}As$ barrier. At low temperatures, carrier relaxation rates are determined mainly by intraband transitions, involving acoustic phonon emission.

The electron-phonon scattering rate $W$for electron transitions from an initial (n,m) to a final (n',m') state with emission of acoustic phonon of energy vq is calculated by the Fermi Golden Rule [6]:

$$\Gamma = \frac{2\pi}{\hbar}\int d^3q\,|M(q)|^2\,\delta(E_{n,m} - E_{n',m'} - \hbar v q). \qquad (1)$$

Here q is the phonon wave vector, v is the longitudinal sound speed, and M (q) is the matrix element for electronic scattering accompanied by the emission of a phonon

$$M(q) = i\pi C(q)[(q_x + iq_y)\delta_{\Delta m=1}G_1 + 2q_z\delta_{\Delta m=0}G_2], \qquad (2)$$

where the overlap integrals are

$$G_1 = \int \rho d\rho dz R_{n',m'}(\rho,z)\rho R_{n,m}(\rho,z), \qquad (3)$$

and

$$G_2 = \int \rho d\rho dz R_{n',m'}(\rho,z) z R_{n,m}(\rho,z). \qquad (4)$$

In the above equations $\Delta m = m - -m$'. $C(q)$ is the coupling constant for piezoelectric (PE) and deformation potential (DP) mechanisms [7], and $R_{n,m}$ are the orbital wave functions, depending upon ρ ($\rho^2 = x^2 + y^2$) and z, and calculated by FEM.

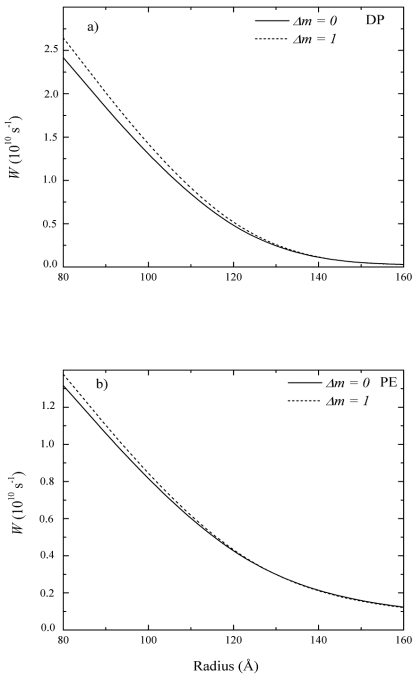

FIG. 1: Electron-acoustic phonon scattering rates as a function of SQD radius for $\Delta m = 0$ (solid line) and $\Delta m = 1$ (dashed line): (a) DP coupling and (b) PE coupling.

Figures 1(a) and 1(b) show the electron-acoustic phonon scattering rates W as a function of the quantum dot radius R for DP and PE mechanisms, respectively. In both situations we consider $B = 0$ T. The data in Figs. 1(a) and (b) are for transitions from the first excited state ($n = 1$, $m = 1$) to the ground state ($n = 0$, $m = 0$) $\Delta m = 1$ (dashed line) and for the transition ($n = 1$, m = 0) to ($n = 0$, $m = 0$) $\Delta m = 0$ (solid line), according to the selection rules given in Eq. (2). In analysing the data in Fig. 1, some interesting aspects can be observed: as the quantum dot radius R increase the rate W decreases for both DP and PE mechanisms. This behaviour is due to the decreasing of electron confinement in the SQD that reduces the value of the overlap integrals and consequently decreases the magnitude of the scattering rates W.

In Fig. 2 (a) and 2 (b) is shown the interface thickness (ξ) influence on the transition rates, for $\Delta m = 1$ (dashed line) and $\Delta m = 0$ (solid line) transitions for $B = 0$ T. We have chosen SQDs of $R = 120$ Å and ξ varying from 0-24 Å. We can realize that for both DP and PE mechanisms, when the interface thickness is increased the electron "feels" a strong spatial confinement leading to a "blue shift" that lift the value of the overlap integrals, increasing the scattering rates W.

When is analysed the influence of an external magnetic field upon the SQD, we can see from Fig. 3 that the scattering rates present a small dependency for $\Delta m = 0$, since electronic levels with $\Delta m = 0$ are weakly perturbed by the applied magnetic field. In opposite, the behaviour of $\Delta m = 1$ transition

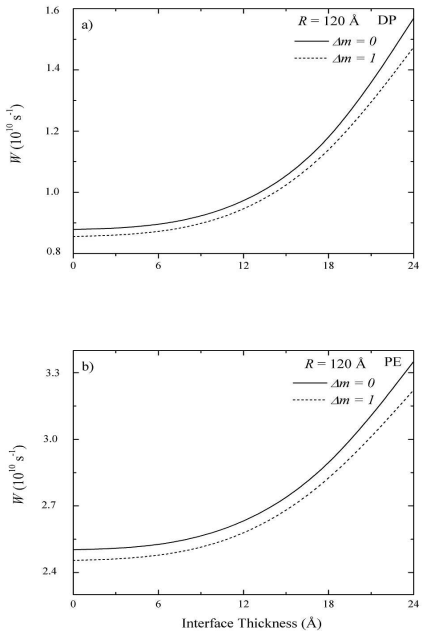

FIG. 2: Electron-acoustic phonon scattering rates as a function of interface thickness for $R = 120$ Å and $\Delta m = 0$ (solid line) and $\Delta m = 1$ (dashed line): (a) DP coupling and (b) PE coupling.

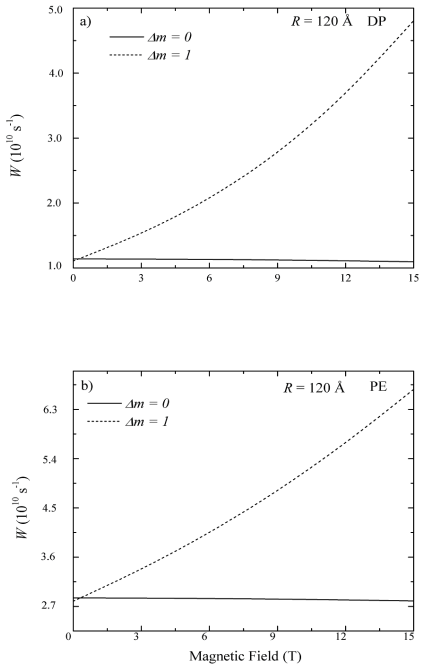

FIG. 3: Electron-acoustic phonon scattering rates as a function of the magnetic field for $R = 120$ Å, $\xi = 18$ Å, $\Delta m = 0$ (solid line) and $\Delta m = 1$ (dashed line): (a) DP coupling and (b) PE coupling.

is strongly modified by external magnetic field, this is due to the extra electron confinement, it is clear that the combination of magnetic and spatial confinements will determine the value of the overlap. In general, when the spatial confinement is strong, the magnetic field produces an additional spatial confinement of the electronic wave functions which is more sensible for Δm = 1 transition. This behaviour, it is clearly showed in Figs. 3 (a) and (b) for both DP and PE mechanisms for a SQD of R = 120 Å, ξ = 18 Å. Solid line and dashed line representing respectively the Δm = 0 and Δm = 1 transitions.

III. CONCLUSION

In conclusion, the effects of a graded interface, SQDs radius and magnetic field upon electron-phonon scattering rates of $Al_xGa_{1-x}As$/GaAs SQDs have been investigated in the frame of FEM. It was found that a roughness interface can strongly modify the rates for both DP and EP mechanism. Further the magnetic field and SQD radius play an important rule for a given Δm= 0, 1 transitions. Indeed, our findings open up new insights for a more precise tuning and control of the carrier dephasing time in semiconductor quantum dots with an impact on device designs.

Acknowledgement

This work has been supported by Fundação de Amparo à Pesquisa do Estado de Minas Gerais (FAPEMIG) and Conselho Nacional de Pesquisa (CNPq).

[1] G. S. Pearson, and D. A Faux, J. Appl. Phys. **88**, 730 (2000).
[2] J. F. Ryan, A. C. Maciel, C. Kiener, L. Rota, K. Turner, J. M. Freyland, U. Marti, D. Martin, F. Morier-Gemoud, and F. K. Reinhart, Phys. Rev. B **53**, R4225 (1996).
[3] Wenhui Duan, Jia-Lin Zhu, and Bing-Lin Gu, Phys. Rev. B **49**, 14403 (1994).
[4] Fanyao Qu, A. M. Alcalde, C. G. Almeida, and N. O. Dantas, J. Appl. Phys. **95**, 2130 (2003).
[5] E. W. S Caetano, M. V. Mesquita, V. N. Freire, and G. A. Faria, Physica E **17**, 22 (2003) and references therein.
[6] P. A. Knipp and T. L. Reinecke, Phys. Rev. B, **52**, 5993 (1995).
[7] The coupling constants $C(q)$ are defined by

$$C_q^{DP} = -i\sqrt{\frac{\hbar}{2\rho_m V\omega_q}}e_q \cdot q\Xi,$$

and

$$C_q^{PE} = \sqrt{\frac{\hbar}{2\rho_m V\omega_q}}e\frac{E^P}{\varepsilon},$$

where $\omega_q = vq$, v is the sound velocity, q is the phonon wave vector. Ξ is the deformation constant, E^P is the piezoelectric constant, ε is the dielectric constant, and ρ_M is the mass density of material. The constants as sound speed, mass density, dielectric constant, and effective mass vary linearly through the interface region. See Wenhui *et al*, Phys. Rev. B, **49**, 14403 (1994) and references therein.
[8] D. R. Santos Jr., Fanyao Qu, A. M. Alcalde, and P. C. Moraes, Physica E, **26**, 331 (2005).