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INFLUENCE OF OPTICAL PHONON CONFINEMENT ON TWO-PHONON CAPTURE PROCESSES IN QUANTUM DOTS

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Electron capture process in GaAs/AlAs spherical quantum dot-quantum well structure is studied theoretically. The capture rate in two polar-optical-phonon-mediated capture processes has been calculated by taking into account the phonon confinement effect. Carrier capture is shown to proceed with rates as high as $10^{10}\,s^{-1}$ at temperature T>100 K. A short capture time is also achieved for low carrier density.

***Keywords*:** capture process, two-phonon processes, confined optical phonons.

The processes involved carrier capture into the dots and intradot relaxation, have been under extensive research during the past decade both experimentally and theoretically. Two different capture and relaxation processes have been considered, via carrier–carrier interaction (Auger processes) or via carrier–phonon coupling [1−4]. The general question of whether or not carrier capture at low carrier densities in a QD structure suffers from phonon bottleneck effects is still hard to answer. Sanguinetti et al. have been presented picosecond time resolved photoluminescence measurements of GaAs/AlGaAs quantum dot structures grown by modified droplet epitaxy, where no wetting layer is connecting the dots and show a fast carrier relaxation time (30 *ps*) to the dot ground state [5]. Most of the nanoscale microcrystallines have a spherical shape. In many cases these spherical QDs are composed of a spherical core of one (core-well) material embedded in a matrix of another (shell-barrier) material.

The inhomogeneous nature of nanostructures leads to strong modifications of the electronic properties as well as the phonon spectrum. The existence of boundaries between the constituting materials and/or the vacuum introduces a coupling of the longitudinal and transverse optical phonon modes even for isotropic media. Additionally, new types of confined (LO1, LO2), interface (IO1, IO2) and surface (SO1, SO2) optical modes can occur in QD-quantum wells [6]. There have been theoretical studies of electron capture [7−9] in QDs due to the various phonon processes: single longitudinal-optical (LO) [7, 8], LO plus acoustic (AC) phonons [8] and two LO phonons [10]. The purpose of the present study is to investigate the effect of phonon confinement on two phonon capture processes in a

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spherical quantum dot-quantum well structure, in the framework of the effective-mass approximation and the rectangular potential barrier model, and derive an expression for the capture rate of electrons for open spherical quantum dots with an arbitrary thickness of barrier layers (from zero to infinity).

We use the one-band approximation for the conduction band electrons and ignore the effects of band mixing, and the electron confinement model by a finite potential well. In the effective mass approximation the Schrödinger equation is solved exactly, resulting to the set of orthonormalized wave functions:

$$\psi_{l,m,n}^{bound}(r,\vartheta,\varphi) = AY_{l,m}(\vartheta,\varphi)\left(j_l(k_0 r)\theta(r_c - r) + \frac{j_l(k_0 r_c)}{h_l^{(+)}(i\kappa r_c)} h_l^{(+)}(i\kappa r)\theta(r - r_c) \right), \quad (1)$$

$$\psi_{l,m,\mathbf{k}}^{unbound}(r,\vartheta,\varphi) = BY_{l,m}(\vartheta,\varphi)\left(j_l(k_1 r)\theta(r_c - r) + \frac{j_l(k_1 r_c)}{f_l(kr_c)} f_l(kr)\theta(r - r_c) \right), \quad (2)$$

where $\psi_{l,m,n}^{bound}$ are the radial wave functions of the discrete spectrum stationary states, the energy levels ($E_{lm} < 0$) of which are defined by the dispersion equation [11]

$$\frac{i\kappa m_1^*}{k_0 m_2^*}\left(\frac{l}{i\kappa r_c} - \frac{h_l'^{(+)}(i\kappa r_c)}{h_l^{(+)}(i\kappa r_c)} \right) = \frac{l}{k_0 r_{cc}} - \frac{j_l'(k_0 r_c)}{j_l(k_0 r_c)}. \quad (3)$$

Here m_1^* and m_2^* denote the effective masses in the dot and the barrier respectively,

$$k_0^2 = 2m_1^* / \hbar^2 (V_0 + E_{lm}), \quad \kappa^2 = -2m_2^* / \hbar^2 E_{lm}, \quad h_l^{(+)}(x) = n_l(x) + ij_l(x), \quad (4)$$

V_0 is the depth of the confining potential well, $j_l(x)$ and $n_l(x)$ are Bessel and Neumann spherical functions, respectively, $\theta(x)$ is the unit step function, $Y_{l,m}(\theta,\varphi)$ are the spherical harmonic functions with $m = 0, \pm 1, ..., \pm s$. $\psi_{l,m,\mathbf{k}}^{unbound}$ are the radial wave functions of the stationary states of the continuous spectrum with the energy $E_{\mathbf{k}} > 0$, and

$$k_1^2 = 2m_1^* / \hbar^2 (V_0 + E_{\mathbf{k}}), \; k^2 = 2m_2^* / \hbar^2 E_{\mathbf{k}}, \quad (5)$$

$$f_l(kr) = \cos(\delta_l) j_l(kr) + \sin(\delta_l) n_l(kr), \quad \tan\delta_l = \frac{kj_l'(kr_c) j_l(k_1 r_c) - k_1 j_l(kr_c) j_l'(k_1 r_c)}{k_1 j_l'(k_1 r_c) n_l(kr_c) - kj_l(k_1 r_c) n_l'(k_1 r_c)}, \quad (6)$$

within the second-order perturbation theory the electron transition probability via emission of two phonons calculated according to [9, 12]

$$W_{IF}^{Two}(\alpha smn, \alpha' s' m' n') = \frac{2\pi}{\hbar}\left| \sum_M \left(\frac{U_{FM}^{em}(\alpha' s' m' n') U_{MI}^{em}(\alpha smn) + U_{FM}^{em}(\alpha smn) U_{MI}^{em}(\alpha' s' m' n')}{E_I - E_M} \right) \right|^2 \times$$
$$\times \delta(E_I - E_F), \quad (7)$$

where $U_{AB}^{em}(\alpha smn)$ is the matrix element of the Hamiltonian for phonon emission. The states involved in the process are labeled as follows: $|I\rangle = |k, i_1, j_1\rangle |\{N_{\alpha smn}^I\}\rangle$ for initial state, $|M\rangle = |t_2, i_2, j_2\rangle |\{N_{\alpha smn}^M\}\rangle$ for intermediate state and $|F\rangle = |t_3, i_3, j_3\rangle |\{N_{\alpha smn}^F\}\rangle$ for final state. The phonon modes are labeled by the quantum number set, as (αsmn). The transition matrix element from $|I\rangle$ to $|M\rangle$ is given by

$$U_{MI}^{em}(\alpha smn) = \sqrt{N_{\alpha smn}^I + 1}\langle t_2, i_2, j_2 | -\Gamma_{sn}^{\alpha}(r) Y_{sm}(\theta,\varphi) | k, i_1, j_1 \rangle, \quad (8)$$

where Γ_{sn} is the radial part of the electron-phonon coupling function [6], N_{smn} is the distribution function of the α type (LO1, LO2, IO1, IO2, SO1, SO2) optical phonons with quantum number set (smn) and frequency $\omega_{\alpha smn}$. The transition matrix element from $|\mathrm{M}\rangle$ to $|F\rangle$ is given by

$$U_{FM}^{em}(\alpha' s' m' n') = \sqrt{N_{\alpha' s' m' n'}^{M}+1}\langle t_3, i_3, j_3 | -\Gamma_{s'n'}^{\alpha'}(r) Y_{s'm'}(\theta,\varphi) | t_2, i_2, j_2 \rangle. \qquad (9)$$

From Eqs. (7)–(9) we obtain

$$W_{IF}(\alpha smn, \alpha' s' m' n') = \frac{2\pi}{\hbar}\Bigg|\sum_{M}\Big(\sqrt{N_{\alpha' s' m' n'}^{M}+1}\sqrt{N_{\alpha smn}^{I}+1}\langle t_2 i_2 j_2 | \Gamma_{sn}^{\alpha}(r) Y_{sm}(\theta,\varphi) | k i_1 j_1 \rangle \times$$
$$\times \langle t_3 i_3 j_3 | \Gamma_{s'n'}^{\alpha'}(r) Y_{s'm'}(\theta,\varphi) | t_2 i_2 j_2 \rangle + \sqrt{N_{\alpha' s' m' n'}^{I}+1}\sqrt{N_{\alpha smn}^{M}+1}\langle t_3 i_3 j_3 | \Gamma_{sn}^{\alpha}(r) Y_{sm}(\theta,\varphi) | t_2 i_2 j_2 \rangle \times$$
$$\times \langle t_2 i_2 j_2 | \Gamma_{s'n'}^{\alpha'}(r) Y_{s'm'}(\theta,\varphi) | k i_1 j_1 \rangle\Big)(E_{k i_1 j_1} - E_{t_2 i_2 j_2} - \hbar\omega_{\alpha smn})^{-1}\Bigg|^2 \times$$
$$\times \delta(E_{k i_1 j_1} - E_{t_3 i_3 j_3} - \hbar\omega_{\alpha smn} - \hbar\omega_{\alpha' s' m' n'}). \qquad (10)$$

The rate (R) of carrier capture from an initial state $|k, i_1, j_1\rangle$ with energy $E_{k i_1 j_1}$ to the QD ground state with energy E_0 by emission of two polar optical phonons within second-order perturbation theory is given by

$$R = \frac{\sqrt{2m}}{4\hbar^2}\sum_{t_3 i_1}\sum_{\substack{\alpha smn,\\ \alpha' s' m' n'}}(N_{\alpha smn}+1)(N_{\alpha' s' m' n'}+1)\sum_{j_1}|Y(sm, s'm', i_1 j_1)|^2 \frac{f(E_{k_0})}{\sqrt{E_{k_0}}} \times$$
$$\times \left|\sum_{t_2}\left(\frac{Q(\alpha sn, \alpha' s' n'; t_3 0, t_2 s', k_{02} i_1)}{E_{k_0} - E_{t_2, s', -m'} - \hbar\omega_{\alpha smn}} + \frac{Q(\alpha' s' n', \alpha sn; t_3 0, t_2 s, k_{02} i_1)}{E_{k_0} - E_{t_2, s, -m} - \hbar\omega_{\alpha smn}}\right)\right|^2 (1 - f(E_0)), \qquad 11)$$

where $f(E_k)$ is the Fermi–Dirac distribution function,

$$E_{k_0} = E_0 + \hbar\omega_{\alpha smn} + \hbar\omega_{\alpha' s' m' n'} \equiv \frac{\hbar^2 k_0^2}{2m}, \qquad (12)$$

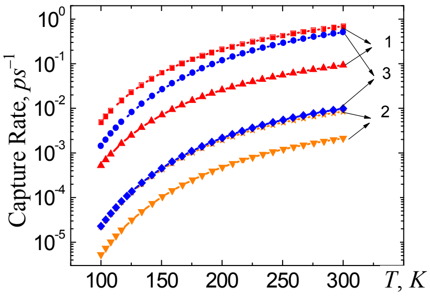
$$Y(sm, s'm', i_1 j_1) = \int_0^{\pi} d\theta \sin\theta \int_0^{2\pi} d\varphi Y_{sm}(\theta,\varphi) Y_{s'm'}(\theta,\varphi) Y_{i_1 j_1}(\theta,\varphi), \qquad (13)$$

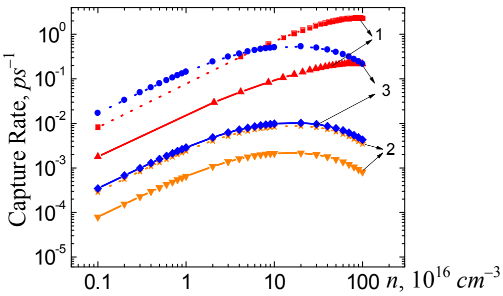
$$Q(\alpha sn, \alpha' s' n'; t_3 i_3, t_2 i_2, t_1 i_1) = \int_0^{\infty} F_{t_2 i_2}^{*}(r)\Gamma_{sn}^{\alpha}(r) F_{t_1 i_1}(r) r^2 dr \int_0^{\infty} F_{t_3 i_3}^{*}(r)\Gamma_{s'n'}^{\alpha'}(r) F_{t_1 i_1}(r) r^2 dr, \qquad (14)$$

$F_{ti}(r)$ are the electron radial wave functions of the stationary states of the discrete and continuous spectrum.

To illustrate possible applications of the theory presented here, we calculated the capture rate as functions of dot radius, temperature and carrier density in GaAs/AlAs spherical quantum dot-quantum well structure. Parameters used for the simulation are: $\varepsilon_{10} = 13.18$, $\varepsilon_{20} = 10.06$, $\varepsilon_{1\infty} = 10.89$, $\varepsilon_{2\infty} = 8.16$ and $\omega_{\mathrm{LO1}} = 36.25$, $\omega_{\mathrm{TO1}} = 33.29$, $\omega_{\mathrm{LO2}} = 50.09$, $\omega_{\mathrm{TO2}} = 44.88\ meV$, $m_{\mathrm{GaAs}} = 0.067 m_0$, $m_{\mathrm{AlAs}} = 0.15 m_0$ [13]. Capture via emission of two phonons has the advantage that it can take place to states with binding energies E_b that fulfill $\hbar\omega_{ph} < E_b \le 2\hbar\omega_{ph}$. In numerical calculations we neglect the interaction with LO2-type phonons, since they are spatially separated from the electron captured in a quantum dot.

The two-phonon emission capture rate dependencies on the lattice temperature for the quantum dot with radius $1.45 a_B$ are presented in Fig. 1. The behavior of the capture rate with temperature follows mainly the behavior of the Bose–Einstein distribution, such that the increase of the capture rate with increasing temperature can be easily obtained. We note that this is in contrast to the findings in [8]. One should note, nevertheless, that the experimentally determined capture rate for InAs/GaAs QD system obviously increases with increasing temperature [14].





1. LO1+LO1 discr.; LO1+LO1 cont.
2. LO1+IO discr.; LO1+IO cont.
3. IO+IO discr.; IO+IO cont.

Fig. 1. Two-phonon capture rate dependence on temperature at a=1.45a_B and carrier densities of 10^{17} cm^{-3}.

Fig. 2. One-phonon capture rate dependence on carrier densities at a=1.45a_B and T=300 K.

The capture rate dependence on carrier density is shown in Fig. 2 for two-phonon capture into the QD ground state. For low carrier densities, the capture rate is very weakly dependent on carrier density. This is because the capture transition rate is proportional to occupation probability of bulk states just beyond the barrier. With an increasing carrier density, the capture transition rate increases at same pace as the bulk part of carrier density. With further increase of carrier density, the states in the dot capable of capturing bulk electrons are becoming populated and cannot participate in capturing and thus the capture rate decreases.

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