PHONON-ASSISTED TRAPPING BY SHALLOW IMPURITIES IN QUANTUM WELLS

Yu. M. Sirenko, V. Mitin, R. Mickevicius, and N. Bannov
Department of Electrical and Computer Engineering,
Wayne State University, Detroit, Michigan 48202

Abstract

The rates of electron trapping and detrapping by shallow donor impurity in the quantum well have been calculated for transitions assisted by the emission and absorption of DA-phonons. For impurities *outside* the infinite square quantum well due to large phonon wave vector the main contribution is given by phonons with a wave vector perpendicular to the well. Numerical calculations give for GaAs and $n_{\mathrm{imp}} \sim 10^{10}/\mathrm{cm}^2$ trapping rates in the range of $10^9 \div 10^{12}/\mathrm{s}$ for electrons on the bottom of the lowest subband. Trapping and detrapping rates decrease rapidly with the increase in electron energy ϵ and are proportional to $(\epsilon + \epsilon_i)^{-7}$, where ϵ_i is an impurity ionization energy.

1 Introduction

The processes of trapping on impurity centers are known to play an important role in transport and noise properties of bulk semiconductors [1]. The capture of bulk carriers by hydrogenic attractive centers is usually treated within a cascade model, where the transitions between the levels of quasi-continuous impurity spectrum occur due to cascade of emitted low-energy acoustical phonons [2]. The trapping of a bulk carrier to a single shallow level of a neutral impurity was considered by Gershenzon *et al* [3]. The capture occurred due to emission of DA-phonon with wave vector Q much greater than other inverse lengths of a problem.

The first consideration of shallow levels of hydrogenic impurities in quantum wells (QW) was performed by Bastard [4] within a variational method. His results have been generalized by a number of authors, far-infrared absorption and photoluminiscence on shallow impurities in QW was studied both experimentally and theoretically.

In this report we study the processes of trapping and detrapping of the electron moving in a QW to a ground state of shallow hydrogenic impurity. In contrast to the case of on-center impurity in a wide QW where *several* bound energy levels can exist and situation resembles that in the bulk, we restrict ourselves to trapping by impurity *outside* the well assuming that electron is captured directly to a *single* bound state. The transitions between the bound and free states are considered to be assisted by emission and absorption of longitudinal DA-phonons.

2 Model and Calculations

Following Bastard [4] we consider the system of the infinite square quantum well of the width W and a shallow donor impurity outside the well. In the effective-mass approximation the unperturbed Hamiltonian of the system is given by

$$\mathcal{H} = \frac{p^2}{2m} - \frac{e^2}{\varepsilon_L \left[\rho^2 + (z - z_i)^2\right]^{1/2}} + V_{QW}(z), \tag{1}$$

where m is an effective mass of electron; ε_L is a lattice dielectric constant; $(0, z_i)$ is an impurity position in cylindrical coordinates, we assume that $z_i \geq W/2$; term $V_{QW}(z)$ is the quantum well potential taken as 0 for $-W/2 \leq z \leq W/2$, and $+\infty$ otherwise.

For the ground state of $\mathcal{H}$ in (1) we use the trial wave function [4] containing variational parameter λ

$$\psi_i(\mathbf{r}) = \frac{N(\lambda)}{\lambda}\, e^{z_i/\lambda}\, e^{-\sqrt{\rho^2+(z-z_i)^2}/\lambda}\, \chi(z). \tag{2}$$

Here $\chi(z) = \sqrt{2/W}\, \cos(\pi z/W)\, \theta(W/2 - |z|)$, where $\theta(x)$ is a step-function, is a transverse wave function of a lowest subband; the normalization coefficient is given by

$$N^2(\lambda) = \frac{2}{\pi}\left[1 + \left(\frac{W}{\pi\lambda}\right)^2\right] \left\{\cosh\frac{W}{\lambda} + \sinh\frac{W}{\lambda}\left[\frac{2z_i}{\lambda} - \frac{2W/\pi^2\lambda}{1+(W/\pi\lambda)^2}\right]\right\}^{-1} \tag{3}$$

Minimization of the expectation value of the Hamiltonian $\mathcal{H}$ for the trial wave function $\psi_i(\mathbf{r})$ gives the value of the variational length λ and ionization energy ϵ_i of the impurity bound state $\epsilon_i = \hbar^2\pi^2/2mW^2 - \langle\psi_i|\mathcal{H}|\psi_i\rangle$.

We consider the transitions between the impurity ground state ψ_i and unperturbed free electron state at the lowest subband (the influence of the impurity potential on the free electron motion is out of consideration) given by

$$\psi_{\mathbf{k}}(\mathbf{r}) = S^{-1/2}\, \exp(i\mathbf{k}\vec{\rho})\, \chi(z), \tag{4}$$

where S is a layer area, and $\mathbf{k} = (k_x, k_y)$ is in-plane electron wave vector.

We treat trapping and detrapping of electrons in QW as transitions between free electron state and ground impurity state due to the interaction with longitudinal DA-phonon modes. For characteristic ionization energies $\epsilon_i \sim 30 \div 100$K, the corresponding phonon momentum will be of the order of Brillouin zone width, as in the case of intervalley scattering. For the calculation of the trapping and detrapping rate we use expressions identical to these for phonon intervalley scattering [6]:

$$W^{\mathbf{Q}}_{\mathbf{k}\to i} = \frac{2\pi}{\hbar}\, N_{\text{imp}}\, \frac{\hbar D^2}{2\rho_L\omega_{\mathbf{Q}}V}\, \left(n_{\mathbf{Q}}+1\right)\, \left|M^{\mathbf{Q}}_{i\to\mathbf{k}}\right|^2\, \delta\left(\epsilon_i + \frac{\hbar^2k^2}{2m} - \hbar\omega_{\mathbf{Q}}\right); \tag{5}$$

$$W^{\mathbf{Q}}_{i\to\mathbf{k}} = \frac{2\pi}{\hbar}\, \frac{\hbar D^2}{2\rho_L\omega_{\mathbf{Q}}V}\, n_{\mathbf{Q}}\, \left|M^{\mathbf{Q}}_{i\to\mathbf{k}}\right|^2\, \delta\left(\epsilon_i + \frac{\hbar^2k^2}{2m} - \hbar\omega_{\mathbf{Q}}\right). \tag{6}$$

Here $W^{\mathbf{Q}}_{\mathbf{k}\to i}$ and $W^{\mathbf{Q}}_{i\to\mathbf{k}}$ are probabilities of transitions between states $\psi_{\mathbf{k}}(\mathbf{r})$ and $\psi_i(\mathbf{r})$ per unit time mediated by short-length phonon with wave vector $\mathbf{Q} = (\mathbf{q}, q_z)$; D is the interaction constant; $\omega_{\mathbf{Q}}$ is a dispersion relation, and $n_{\mathbf{Q}}$ is a phonon occupancy number; ρ_L and V are crystal density and volume. The quantity $M^{\mathbf{Q}}_{i\to\mathbf{k}}$ is a marix element of transition; with allowance for Eqs. (2) and (4) after integration over the polar angle we obtain:

$$M^{\mathbf{Q}}_{i\to\mathbf{k}} \equiv \left\langle\psi_{\mathbf{k}}\left|e^{i\mathbf{Qr}}\right|\psi_i\right\rangle = \frac{2\pi N(\lambda)}{\lambda S^{1/2}}\, e^{z_i/\lambda} \int_{-W/2}^{W/2} dz\, \chi^2(z)e^{iq_zz} \int_0^\infty \rho d\rho\, e^{-\sqrt{\rho^2+(z-z_i)^2}/\lambda}\, J_0(|\mathbf{q}-\mathbf{k}|\rho). \tag{7}$$

To calculate the rate of trapping (detrapping) from (to) the state with given $\mathbf{k}$ we have to perform the summation in Eqs. (5) and (6) over all possible bulk phonon wave vectors $\mathbf{Q}$. Energy δ-function specifies the magnitude of phonon wave vector. For given impurity ionization energy ϵ_i and electron energy $\epsilon = \hbar^2k^2/2m$ the magnitude Q_ϵ of phonon wave vector is defined by the energy conservation law:

$$\hbar\omega_{Q_\epsilon} = \epsilon_i + \epsilon. \tag{8}$$

In the following we restrict ourselves by the case of such energies ϵ_i and ϵ that phonon wave vector Q_ϵ is much greater than other values of the same dimensionality. This is a realistic approximation for characteristic lengths of the order of hundred angstroms and $\epsilon_i + \epsilon \geq 20$ K. In this case due to rapidly oscillating factors $\exp(iq_z z)$ and $J_0(|\mathbf{q}-\mathbf{k}|\rho)$ in Eq. (7) the trapping and detrapping rates decrease rapidly with the increase of Q. Analysis of the integral in Eq. (7) shows that for finite values of $|z - z_i|$ (i.e. impurity *outside* infinite square well) the matrix element $M^{\mathbf{Q}}_{i\to\mathbf{k}}$ decreases exponentially with $|\mathbf{q}-\mathbf{k}|$ and only algebraically with q_z. Therefore emission (absorption) of phonons with longitudinal momentum component $\mathbf{q}$ differing much from electron momentum $\mathbf{k}$ is unfavorable ("quasi-conservation" of momentum in xy-plane) and *main contribution* to trapping and detrapping of electrons is given by *"transverse" phonons* with

$$Q \approx q_z \gg q, k.$$

The situation would be different for the case of in-channel impurity or the impurity outside the well of a finite height, where the contribution of phonons with small and large longitudinal components q can be comparable and would resemble the trapping of electrons in the bulk by the neutral impurities [3].

Substituting the expression (7) for matrix element into Eqs. (5) and (6) and performing the integration over phonon wave vector $\mathbf{Q}$ we find, with the help of identity $\int_0^\infty x dx\; J_0(x\rho)\; J_0(x\rho') = \delta(\rho - \rho')/\rho$, the following expressions for the differential trapping and detrapping rates:

$$W_{tr}(\epsilon) = n_{\rm imp}\,\frac{D^2}{\rho_L}\left|\frac{d\omega_{Q_\epsilon}}{dQ}\right|^{-1}\frac{n_{Q_\epsilon}+1}{\epsilon_i+\epsilon}\;\frac{\mathcal{F}}{2\pi^2\,(Q_\epsilon W/2\pi)^6}; \tag{9}$$

$$\frac{dW_{detr}(\epsilon)}{d\epsilon} = \frac{m}{2\pi\hbar^2}\,\frac{D^2}{\rho_L}\left|\frac{d\omega_{Q_\epsilon}}{dQ}\right|^{-1}\frac{n_{Q_\epsilon}}{\epsilon_i+\epsilon}\;\frac{\mathcal{F}}{2\pi^2\,(Q_\epsilon W/2\pi)^6}; \tag{10}$$

Here $W_{tr}(\epsilon)$ is the probability per unit time for electron with energy ϵ to be trapped; $dW_{detr}(\epsilon)/d\epsilon$ is the probability per unit time for trapped electron to be ionized to the interval of energies from ϵ to $\epsilon + d\epsilon$; $n_{\rm imp} = N_{\rm imp}/S$ is a sheet impurity density; $d\omega_Q/dQ$ is a derivative of phonon spectrum, for small Q it tends to the sound velocity; factor $\mathcal{F}$ is given by

$$\mathcal{F} = N^2(\lambda)\,\left[\left(1+\frac{2z_i}{\lambda}\right)\cosh\frac{W}{\lambda} - \frac{W}{\lambda}\sinh\frac{W}{\lambda} - \Omega\cos Q_\epsilon W\right], \tag{11}$$

where $\Omega = \lambda^{-2}\int_0^\infty \rho d\rho\, \exp\left[-\sqrt{\rho^2+(z_i+W/2)^2}/\lambda\right]\,\exp\left[-\sqrt{\rho^2+(z_i-W/2)^2}/\lambda\right]$ is amplitude of the oscillations in trapping and detrapping rate owing to the of sharp edge in transverse electron wave function. Note, that Ω is always smaller than nonoscillatory terms in Eq. (11). Detailed analysis of other limiting cases shows that the approximation of large phonon wave number Q used in deriving Eqs. (9) – (11) is good for $Q_\epsilon W \geq 2\pi$.

Besides the differential trapping and detrapping probabilities $W_{tr}(\epsilon)$ and $dW_{detr}(\epsilon)/d\epsilon$ we will consider also integral characteristics:

$$1/\tau_{tr} = \int_0^\infty f(\epsilon) W_{tr}(\epsilon)\; d\epsilon\;; \tag{12}$$

$$1/\tau_{detr} = \int_0^\infty \left[1 - \frac{\pi\hbar^2 n_e}{m}\, f(\epsilon)\right]\,\frac{dW_{detr}(\epsilon)}{d\epsilon}\, d\epsilon\;. \tag{13}$$

Here τ_{detr} and τ_{tr} are lifetimes of occupied and unoccupied state of a given impurity; $f(\epsilon)$ and n_e are the distribution function and concentration of electrons on a lowest subband. Trapping-detrapping balance equation allows to determine for given times τ_{detr} and τ_{tr} the concentration of the trapped electrons, $n_{\rm tr} = n_{\rm imp}\;\tau_{detr}/\left(\tau_{detr} + \tau_{tr}\right)$.

3 Numerical Results

We evaluate the trapping and detrapping rates $W_{tr}(\epsilon)$ and $dW_{detr}(\epsilon)/d\epsilon$ given by Eqs. (9) – (11) for the parameters of GaAs; we used the value $D = 10^9$ eV/cm for short-wave DA-phonon interaction constant [5]. Sheet impurity concentration was chosen to be $n_{imp} = 10^{10}/\mathrm{cm}^2$; electron concentration on the lowest subband $n_e = 10^{11}/\mathrm{cm}^2$; electrons and phonons were assumed to be in equilibrium with temperature $T_e = T_{ph} = 300$ K.

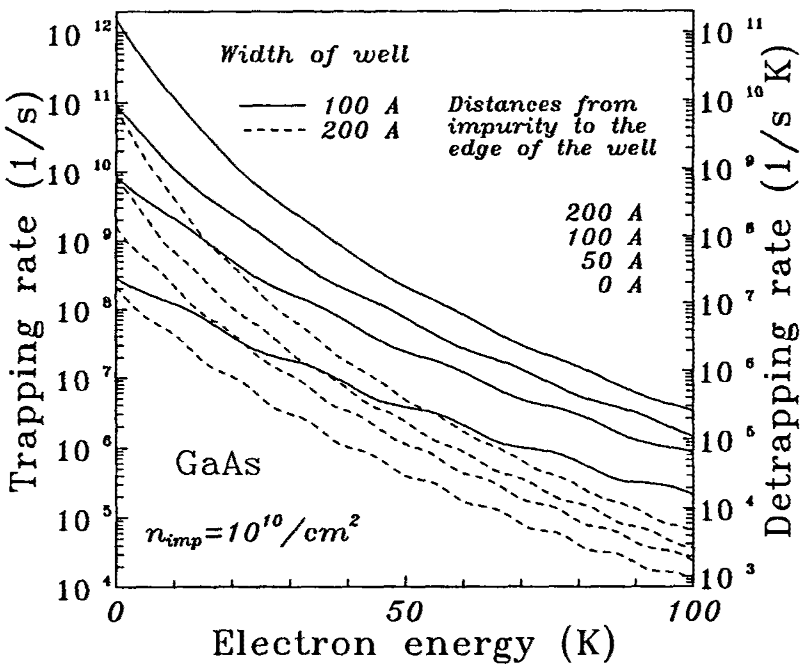

Figure. Trapping $W_{tr}(\epsilon)$ (left axis) and detrapping $dW_{detr}(\epsilon)/d\epsilon$ (right axis) differential rates versus electron energy ϵ.
Solid lines. Well width $W =$ 100 Å; from the bottom to the top: impurity position z_i = 50, 100, 150, 250 Å; ionization energy ϵ_i = 70, 47, 36, 25 K; variational length λ = 156, 209, 254, 331 Å.
Dashed lines. Well width W = 200 Å, from the bottom to the top: impurity position z_i = 100, 150, 200, 300 Å; ionization energy ϵ_i = 44, 35, 28, 21 K; variational length λ = 225, 267, 305, 373 Å.

On the figure we present the results of evaluation of $W_{tr}(\epsilon)$ and $dW_{detr}(\epsilon)/d\epsilon$ for several sets of parameters W and z_i. Calculated trapping and detrapping rates decrease rapidly with the increase in electron energy, being proportional to $(\epsilon_i + \epsilon)^{-7}$. Impurities at large distance z_i have smaller ionization energies and therefore lead to greater trapping rates than on-edge impurities.

The integral trapping and detrapping rates calculated with the help of Eqs. (12) and (13) are in the range from $\tau_{tr} = 4.9 \times 10^{-8}$ s and $\tau_{detr} = 7.8 \times 10^{-9}$ s (for W = 200 Å and z_i = 100 Å) to $\tau_{tr} = 1.0 \times 10^{-11}$ s and $\tau_{detr} = 1.6 \times 10^{-12}$ s (for W = 100 Å and z_i = 250 Å), corresponding concentration of captured electrons is about $n_{tr} = (0.14 \div 0.19)\ n_{imp}$.

Calculated rates of trapping and detraping will be included in Monte Carlo codes to investigate the effect of capture on noise and transport properties of carriers in quantum wells.

This work is supported by the National Science Foundation under grant #NSF ESC-9110705.

References

[1] L. Reggiani and V. Mitin, Rivista del Nuovo Cimento, **12**, 1 (1989).
[2] V. N. Abakumov, V. I. Perel, and I. N. Yassievich, Sov. Phys. Semicond., **12**, 1 (1978).
[3] E. Gershenzon, G. Goltsman, G. Ptitsina, and N. Riger, Sov. Phys. JETP, **64**, 889 (1986).
[4] G. Bastard, Phys. Rev. **B24**, 4714 (1981).
[5] L. Reggiani, *Hot Electron Transport in Semiconductors*, in *Topics in Applied Physics*, Vol. 58 (Springer-Verlag, Berlin, Heidelberg, 1985).