

# Substantial contribution of effective mass variation to electron-acoustic phonon interaction via deformation potential in semiconductor nanostructures

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Using the approach of deformed ions and the tight binding, we have demonstrated that the interaction of electrons confined in a nanostructure with acoustic phonons in a cubic crystal is described by a deformation potential tensor (DPT) whose symmetry is determined by the geometry of the nanostructure. Here in, we present additional contribution to the DPT which is caused by the deformation dependence of the electron effective mass and it increases as  $L^{-2}$  when the characteristic size of a nanostructure,  $L$ , decreases. For narrow GaAs-based quantum wells, this contribution is comparable with and can overcome that from the usual deformation potential coupling. © 1999 American Institute of Physics. [S0003-6951(99)00911-0]

Interaction via the deformation potential (DP) is one of the most important mechanisms of the coupling between electrons and acoustic vibrations in semiconductors. For a homogeneous semiconductor of the cubic crystal symmetry with a conduction band minimum at the  $\Gamma$  point, the interaction Hamiltonian is given by<sup>1</sup>

$$H_{\text{int}} = D \operatorname{div} \mathbf{u}, \quad (1)$$

where  $D$  is the deformation potential constant, and the divergence of the lattice displacement,  $\mathbf{u}$ , determines the relative change of crystal volume due to deformation. In the framework of the effective-mass approximation, the theory of DP has been shown to be valid for slowly varying (on the scale of the lattice period) deformations.

At low temperatures, DP interaction plays an important role in the kinetics of confined electrons. It determines the phonon limited mobility and energy losses of a two-dimensional (2D) electron gas<sup>2</sup> and acoustic-phonon emission may be the only process responsible for electron energy relaxation in dot structures.<sup>3</sup> The accepted procedure in the calculation of the deformation interaction in semiconductor heterostructures is to use the bulk interaction Hamiltonian of Eq. (1). It is assumed that the parameter  $D$  does not depend on a size and a shape of the quantum heterostructure. Only acoustic field modifications which result from the difference in the elastic properties of materials forming the heterojunctions are taken into account.<sup>4</sup> Recently, a new mechanism of electron-acoustic phonon interaction, which is intrinsic to semiconductors that have interfaces, and is additional to usual deformation potential coupling of Eq. (1), has been considered.<sup>5,6</sup> It arises when acoustic waves cause the interface spacing to change and thereby to perturb the electron states. This additional interaction,<sup>5</sup> known as “macroscopic deformation potential” (MDP), for electrons occupying the

lowest subband of a rectangular quantum well (QW) has been written in the form

$$H_{\text{int}}^{\text{MDP}} = \frac{2E_1}{L} [u_z(x, y, 0) - u_z(x, y, L)], \quad (2)$$

where  $E_n = \pi^2 \hbar^2 n^2 / 2m^* L^2$ ,  $m^*$  is the isotropic effective mass, and the planes  $z=0$  and  $z=L$  are at the positions of the interfaces. An interaction of the same nature, known as the “ripple mechanism” (RM), which is applicable for all nanostructure geometries, was introduced by<sup>6</sup>

$$H_{\text{int}}^{\text{RM}} = \mathbf{u}(\mathbf{r}) \nabla U(\mathbf{r}), \quad (3)$$

where  $U(\mathbf{r})$  is a confinement potential. In contrast to the case of the bulk mechanism of Eq. (1), which allows only the interaction with longitudinal phonons in isotropic media, transverse acoustic phonons contribute to the interactions of Eqs. (2) and (3) as well. The MDP interaction is weak compared with the bulk interaction of Eq. (1) as  $2E_1/D \ll 1$ . For small dot sizes, it was found<sup>6</sup> that the RM contribution to the electron scattering rates can be larger than that from Eq. (1).

The finite-size effect in quantum heterostructures is not limited to the MDP (or RM) interaction. The deformation variation of the electron effective mass also gives rise to a size-dependent contribution. Let us consider a change of electron energy in a rectangular QW, under an applied uniaxial strain: the displacement  $u(z) = -\gamma z$  with  $\gamma = \text{const}$ . Pressure is accommodated by shifting of the zone-center energy of the bulk semiconductor according to Eq. (1), and by shifting of the energy levels in the QW. Taking into account the change of  $E_1$  both due to  $L(\gamma) = L(0)(1 - \gamma)$  and  $m^*(\gamma) = m^*(0)(1 + \gamma\chi)$ , where  $\chi$  is a phenomenological parameter, in the first order of  $\gamma$  we get the overall energy shift

$$\delta E = \gamma [-D + (2 - \chi)E_1]. \quad (4)$$

Here the term  $2\gamma E_1$  coincides with  $H_{\text{int}}^{\text{MDP}}$ . The sign of this shift corresponds to that of the relative change of QW width:

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in the case of compression,  $\gamma > 0$ , the energy level moves up [the perturbation of Eq. (3) gives  $-2\gamma E_1$ ]. For electrons with three-dimensional (3D) wave vector,  $\mathbf{k}$ , the contribution of the pressure dependence of  $m^*$  to shifting the electron energy is proportional<sup>7</sup> to  $k^2$ , and the effect is negligible for energies near band edge ( $\mathbf{k} \rightarrow 0$ ). In the case of heterostructures, the minimum of the electron energy is determined by the finite energy of spatial quantization, and this contribution is not small. To estimate this effect, one can express  $\chi$  through the slope  $dE_g/dP$  of the pressure band gap energy dependence, which is measured experimentally under an applied hydrostatic pressure. Using the known expressions for  $m^*$  from  $\mathbf{k} \cdot \mathbf{p}$  perturbation theory, in the case when the interaction of nearest nondegenerate bands is substantial, one obtains for relative changes the relationship<sup>7</sup>  $\delta m^*/m^* \approx \delta E_g/E_g$ . Taking into account that the value of  $\chi$  in Eq. (4) corresponds to a uniaxial (not hydrostatic) pressure, we obtain

$$\chi \approx \frac{3K}{E_g} \frac{dE_g}{dP}, \quad (5)$$

where the quantitative  $K$  is the modulus of the hydrostatic compression. Using the data given in Ref. 8, we find  $\chi \approx 17$  for GaAs and  $\chi \approx 40$  for InAs. We see that this contribution may exceed that given by the MDP (or RM) mechanism. For narrow QWs it can be comparable with the energy shift via the bulk deformation potential. For a GaAs-based QW with a width  $L = 10$  nm, one obtains  $(\chi - 2)E_1 = 0.84$  eV, i.e., about 10% of  $D$  value. This contribution increases as  $L^{-2}$  when  $L$  decreases. If the signs of  $D$  and  $\chi$  are different, then the electron-acoustic phonon interaction in a QW is to be weaker than that from the bulk DP interaction.

In Eq. (4), which predicts the energy shift induced by homogeneous deformation, the size-dependent part enters additively and is described by  $E_1(L)$ . For the case of interaction with acoustic waves, the displacement  $\mathbf{u}(\mathbf{r})$  can be altered on the scale of an interface spacing. It gives additional dependencies of the energy shift on  $L$  which are different for the interface mechanisms and bulk interaction of Eq. (1). In the present work, to derive the electron-acoustic phonon interaction Hamiltonian which describes the DP interaction and the overall contribution of the interfaces we start from the microscopic level. In this way, the assumption about independent contributions of the different mechanisms under considerations is not used.

Consider an electron with the free mass,  $m_0$ , in a crystal with the lattice potential,  $V(\mathbf{r})$ . To determine the perturbation caused by a smooth displacement,  $\mathbf{u}(\mathbf{r})$ , we use the model of deformed ions. According to this model, the lattice potential in a deformed crystal equals  $V(\mathbf{r} - \mathbf{u})$ . The change of the potential,  $V(\mathbf{r} - \mathbf{u}(\mathbf{r})) - V(\mathbf{r})$ , upon using a Taylor expansion for small acoustic displacements, yields

$$H_{\text{int}} = -(\mathbf{u}(\mathbf{r}) \cdot \nabla) V(\mathbf{r}). \quad (6)$$

We will neglect the modification of elastic parameters in heterostructures and will use bulk-like expressions for the displacement:  $\mathbf{u} = \mathbf{e} u_0 \exp(i\mathbf{q}\mathbf{r})$ , where  $\mathbf{e}$  is a polarization unit vector,  $\mathbf{q}$  is a 3D wave vector, and  $u_0$  is an appropriately

normalized amplitude. In this approach, the presence of interfaces in Eq. (6) is accounted for entirely by the lattice potential.

Consider first a 2D electron layer bounded by  $0 \leq z \leq L$ . Introducing the periodic boundary conditions in the  $xy$  plane containing  $N_x N_y$  elementary cells, one can write the eigenfunctions in the undeformed crystal as

$$\Psi_{n\mathbf{k}} = (N_x N_y)^{-1/2} e^{i\mathbf{k}\mathbf{r}} \psi_{n\mathbf{k}}(\mathbf{r}), \quad (7)$$

where  $\mathbf{k} = (k_x, k_y)$  stands for the 2D electron wave vector,  $\psi_{n\mathbf{k}}(\mathbf{r})$  is a periodic function over  $x$  and  $y$  with the lattice period, and describes the localized states in the  $z$  direction ( $n = 1, 2, \dots$ ,  $\psi_{n\mathbf{k}}(\mathbf{r}) = 0$  at  $z = \pm \infty$ ). The matrix element of the intrasubband transitions between the states  $n\mathbf{k}$  and  $n\mathbf{k}'$  is

$$M_{n\mathbf{k}', n\mathbf{k}} = -iu_0 \int_{-\infty}^{\infty} dz \int d\rho e^{iq_z z} \psi_{n\mathbf{k}}^* \psi_{n\mathbf{k}} e^{iq_z z} (\mathbf{e} \cdot \nabla) V(\mathbf{r}). \quad (8)$$

Here  $\mathbf{k}' = \mathbf{k} + \mathbf{q}_{\parallel}$ ,  $\mathbf{q}_{\parallel} = (q_x, q_y)$ ,  $\rho = (x, y)$ , the integral over  $x, y$  is spread over one elementary cell. Using the Green identity and then the Schrödinger equation for  $\psi_{n\mathbf{k}}$ , one can eliminate  $V$  from Eq. (8). For transitions near the bottom of the subband, we get

$$M_{n\mathbf{k}', n\mathbf{k}} = -i \frac{\hbar^2}{m_0} u_0 \int_{-\infty}^{\infty} dz \int d\rho e^{iq_z z} \left[ \frac{1}{2} (\mathbf{e} \cdot \mathbf{q}_{\parallel}) |\nabla_{\parallel} \psi_{n0}|^2 + e_z q_z |\nabla_z \psi_{n0}|^2 \right], \quad (9)$$

where  $\psi_{n0} \equiv \psi_{n\mathbf{k}=0}$ . Here and in the remainder of this letter, a change of  $\mathbf{u}(\mathbf{r})$  within an elementary cell is neglected. Replacing  $\psi_{n\mathbf{k}}$  with  $\psi_{n0}$ , we neglect the contribution caused by a change of  $m^*$  in the  $x, y$  plane. To calculate the functions  $\psi_{n0}$ , we exploit a tight-binding approach in a crystal with a simple cubic lattice and assume that only first-neighbor cell couplings are nonzero. For a slab which consists of  $N$  cells in the (001) direction, the electron wave functions are given by<sup>9</sup>

$$\psi_{n0}(\mathbf{r}) = \left( \frac{2}{N+1} \right)^{1/2} \sum_l \sin \left( \frac{\pi n l_z}{N+1} \right) \varphi_l(\mathbf{r}), \quad (10)$$

where  $\varphi_l = \varphi(\mathbf{r} - b\mathbf{l})$  is a state of an isolated  $l$ th cell, and  $b$  is the lattice period,  $l_z = 1, 2, \dots, N$ . Let the "atomic" function  $\varphi(\mathbf{r})$  be the electron ground state in 3D rectangular quantum dot with the potential  $V=0$  for  $-a/2 < x, y, z < a/2$  and  $V = V_0$  outside the well. We assume that  $\kappa a \gg 1$  ( $\kappa = \sqrt{2m_0 V_0 / \hbar^2}$ ). Using a multiplicative form,  $\varphi(\mathbf{r}) = \varphi_x(x) \varphi_y(y) \varphi_z(z)$ , where  $\varphi_x(x)$  is a state in a one-dimensional QW, we get (for  $\pi n / N \ll 1$ )

$$M_{n\mathbf{k}', n\mathbf{k}} = iu_0 [(\mathbf{e} \cdot \mathbf{q}) D + e_z q_z (2 - \chi) E_n] F_{nn}, \quad (11)$$

$$F_{nn'} = \frac{2}{L} \int_0^L \sin \frac{\pi n z}{L} \sin \frac{\pi n' z}{L} dz.$$

Here the deformation potential is

$$D = -\frac{\pi^2 \hbar^2}{a^2 m_0} (1 - 4(d/a) e^{-\kappa d}), \quad (12)$$

and the deformation dependence of  $m^*$  is determined by  $\chi = -\kappa d$ , where  $d = b - a$  is the interwell barrier width, and  $\kappa d \gg 1$  [in this model,  $1/m^*$  is proportional to  $\exp(-\kappa d)$ ].

From Eq. (11) it follows that the intrasubband scattering of 2D electron gas in a cubic crystal is described by interaction Hamiltonian  $H_{\text{int}} = D_{ij}u_{ij}$ , where  $u_{ij}$  is a strain tensor,  $D_{ij}$  is the diagonal tensor of deformation potential which has the components  $D_{xx} = D_{yy} = D$ ,  $D_{zz} = D + (2 - \chi)E_n$ . The above used microscopical model of a crystal can be easily generalized on the two- and three-dimensional confinement potentials. In the general case, the symmetry of the tensor  $D_{ij}$  is determined by the geometry of the nanostructure.

Consider the finite-size effect in the interlevel transitions in cubical quantum dots. For an infinite potential outside of the dot, the electronic energies are  $E_n = [(\pi^2 \hbar^2)/(2m^*L^2)] \times (n_x^2 + n_y^2 + n_z^2)$ , where  $(n_x, n_y, n_z)$  equals (111) for the ground state, and  $(n_x, n_y, n_z)$  equals (211), (121), or (112) for the threefold-degenerate first-excited state. A straightforward calculation of the matrix element,  $M_{12}$ , of transitions from the state (112) to the state (111), gives

$$M_{12} = iu_0[(\mathbf{e} \cdot \mathbf{q})(D + \chi E_1) + e_z q_z (3\chi/2)E_1]F_{11}(q_x)F_{11}(q_y)F_{12}(q_z), \quad (13)$$

where  $D$  and  $\chi$  have the same definitions as in Eq. (11) (with allowance of inequality  $\kappa d \gg 1$ , we have neglected small terms which describe the RM contribution). In Eq. (13), due to the energy conservation law, the phonon wave vector,  $q_z$ , is considerably larger than the inverse dot size  $1/L$ . On the other hand, the theory is valid if  $q_z$  is small compared to the inverse lattice constant,  $1/b$ . These two criteria may be satisfied only for large-size dots ( $L > 50$  nm for GaAs-based structures). In this case, the correction terms,  $\chi E_1$ , in Eq. (13) are negligibly small.

In conclusion, we have demonstrated the role of the deformation dependence of the electron effective mass in the

interaction of electrons with acoustic phonons in quantum heterostructures. Starting from microscopic consideration, we have derived a part of the interaction, which describes the interfaces' contribution. It was shown that the deformation dependence of the effective mass contributes a size-dependent part to the electron-acoustic phonon interaction. This contribution can exceed that from the mechanism<sup>5,6</sup> which originates from the phonon-induced vibrations of heterointerface boundaries. Unlike the usual deformation interaction in cubic crystals, this mechanism as well as the mechanism of Refs. 5 and 6 may involve electron interaction with transverse acoustic phonons. For narrow QWs, the interaction with longitudinal acoustic modes due to this mechanism is comparable to and may overcome that from the bulk deformation potential. The results obtained in the framework of the tight-binding approximation show that interlevel transitions in quantum dots larger than 50 nm are well described by the usual bulk deformation potential.

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