Study of acoustical phonon modes in superlattices with SiGe QDs

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The results of a theoretical study of the phonon spectrum of crystal structures with quantum dots are reported. The model proposed takes into account the real crystal structure of both the quantum dots and surrounding matrix. A comparison is made for the numerically calculated and experimental Raman spectrum of a multilayer Ge/Si QD structure, which shows a qualitative correlation between the theory and experiment.

1   Introduction

The crystal structures containing quantum dots (QD) or quantum wires have been studied by spectroscopic methods during more then ten years. Significant efforts are directed to understand the spectral features in dependence on the size of QDs imbedded into a matrix, their concentration and ordering.

One of the first works on this problem was connected with CdSe nanospheres [1] which were considered in the framework of classical models: semiconductor homogenious nanosphere of radius R having a dielectric constant ε and imbedded into matrix with dielectric constant ε_d. The following steps were connected with the study of Raman scattering (RS) by self-assembled quantum dots (QD) based on more real models. First RS study was limited by optical phonon frequency range [2, 3] but the following intensive investigations were related to the RS on acoustical phonons. In the experiments the periodic oscillations were observed (see for example [4-6]) and attributed to the interaction between confined electronic states and standing acoustic waves due to reflection at the sample surface. Model calculations were made by using the deformation potential interaction between acoustical phonons and electronic states confined within the QD. The calculations allowed authors of [6] to make conclusion that oscillations in RS spectrum are related to interference between the QD layers. However, such a conclusion seems to be very surprising because for the interference to occur, it is necessary that path difference d for two interacting waves must have a value comparable to the probing wavelength λ, $(d \geq \lambda)$. In fact, the distance between two QD layers is much smaller ($d \approx 0.1\lambda$). In accordance to model proposed in [5,6], QD's are homogeneous disks including the in-plane and vertical confinement. Acoustic phonons in each layer have appropriate velocities and densities, $v_{QD}, \rho_{QD}, v_{Si}, \rho_{Si}$, (the details of model are presented in [7]). According to [7], the electronic confinement leads to the loss of translational invariance and RS by acoustic phonons becomes allowed.

Really, authors of this and other similar models neglect the fact that QD has 30-50 nm in lateral and 3-15 nm in vertical size. Taking into account that Si and Ge crystal lattice constant is near ~0.5 nm, QD contains many crystal unit cells. It allows, if one neglects Si/Ge lattice mismatch of about 4%, to build the new unit cell containing Ge QD and part of surrounding Si matrix, as schematically shown in Fig.1. The lattice parameters of the new cell are obtained from the original (old) ones as follows : $a \rightarrow La, L = \{L_x, L_y, L_z\}$.
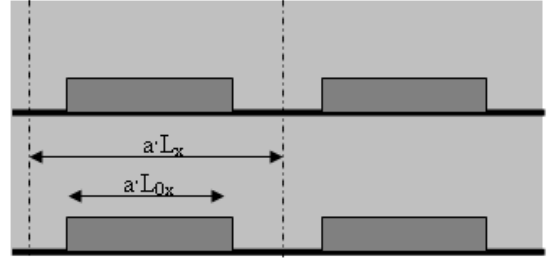

Fig. 1. Schematic of the new unit cell in the QD structure. L_x is a number of the old unit cells in a new unit cell; L_{0x} is a number of the old unit cells of QD.

Such model with "new crystal structure" allows analysis of the RS features in framework of micro-approach, using only traditional parameters of real crystals (phonon frequency, mass of atoms, lattice constant etc.). It is obvious that a number of optical phonon branches will increase because the new reciprocal lattice vector, b_L, is smaller then the former one, b, ($b = 2\pi / a \rightarrow b_L = 2\pi / La$). Each primary optical branch is transformed into several optical and each acoustical branch is transformed into several optical and one acoustical branches (sometimes such transformation is called as folding of phonon branch). Therefore the structure of low frequency bands will result from the appearance of many new optical phonons but not from of the interference effect on RS.

2   Short theory

2.1   Energy of crystal

Energy of the crystal consists of the energy of electron system, H_{el}, energy of vibrations, H_{ph}, and energy of electron-phonon interaction $H_{el=ph}$. We will consider in this article the processes of non-resonance Raman scattering, therefore it is sufficient to take into consideration only the phonon part of the Hamiltonian. Within a harmonic approximation, the energy of lattice vibrations can be written in traditional form:

$$E = T + V = \frac{1}{2} \sum_{\tilde{n},\alpha,k} m_k (\dot{u}_{\tilde{n},\alpha}^k)^2 +$$

$$+ \frac{1}{2} \sum_{\substack{\tilde{n},\alpha,k \\ \tilde{n}',\alpha',k'}} V(\tilde{n},\alpha,k,\tilde{n}',\alpha',k') u_{\tilde{n},\alpha}^k u_{\tilde{n}',\alpha'}^{k'} . \qquad (1)$$

In Eq.(1) $u_{\tilde{n},\alpha}^k$ characterizes the deviation of the position of atom k (with mass m_k) in unit cell n along axis $\alpha = \{x, y, z\}$ from equilibrium position; $\dot{u}_{\tilde{n},\alpha}^k$ is the corresponding velocity.

We will consider the crystal with QDs as schematically shown in Fig. 1. Note that the model developed for QD's can be easily adapted for the case of quantum wires by setting $L_{0x} = L_x$ or quantum wells by setting $L_{0x} = L_x$, $L_{0y} = L_y$. The part of unit cells, included in the new unit cell, can be occupied by atoms of one type of crystal (for example, Ge, GaAs etc.) and another one is occupied by atoms of other crystal (Si, AlAs etc.). Therefore the both sums in the Eq.(1) can be transformed to unite unit cells only with atoms of one type of crystal and rest is terms of mixed type. The procedure of such re-summation is to some degree cumbersome, especially for the second term in Eq.(1). As we neglect QD/matrix lattice mismatch, we can introduce a new great unit cell with a constant $a \rightarrow La$. Then the position of unit cells will be characterized by two indeces $\tilde{n} = \{N, n\}$ and small unit cell should be marked by index 0, if it belongs to QD, and index 1, if it belongs to matrix, i.e. $n \rightarrow n_0, n_1$, but for great unit cell which contain only one type material $n_0 + n_1 = n$. Beside it would be convenient to use in all analytical expressions the parameters of great init cell ($L = \{L_x, L_y, L_z\}$) and to make the summation either on great unit cell or only on unit cells connected with QD to avoid the complex geometrical form connected with surrounding matrix. Therefore the Eq.(1) can be rewritten in other form (it is shown below for kinetical part of energy) to pick out the terms corresponding to energy of the full crystalconsisting either only of QD material or only of matrix material and the rest terms are perturbation ones (the full number of unit cells in crystal is $\tilde{N} = NL$).

$$T = \frac{1}{2} \sum_{N, n_1, \alpha, k} m_k^1 (\dot{u}_{n_1, \alpha}^{1, k})^2 + \frac{1}{2} \sum_{N, n_0, \alpha, k} m_k^0 (\dot{u}_{n_0, \alpha}^{0, k})^2 =$$

$$= \{ \frac{1}{2} \sum_{N, n, \alpha, k} m_k^1 (\dot{u}_{n, \alpha}^{1, k})^2 - \frac{1}{2} \sum_{N, n_0, \alpha, k} m_k^1 (\dot{u}_{n_0, \alpha}^{1, k})^2 \} +$$

$$+ \frac{1}{2} \sum_{N, n_0, \alpha, k} m_k^0 (\dot{u}_{n_0, \alpha}^{0, k})^2 = \{ T^{(1)} - \frac{1}{2} \sum_{N, n_0, \alpha, k} m_k^1 (\dot{u}_{n_0, \alpha}^{1, k})^2 \} +$$

$$+ \{ T^{(0)} + [-T^{(0)} + \frac{1}{2} \sum_{N, n_0, \alpha, k} m_k^0 (\dot{u}_{n_0, \alpha}^{0, k})^2] \}, \qquad (2)$$

where $T^{(0)}$ and $T^{(1)}$ are kinetic energy of vibrations of the whole crystal which consists of the material of quantum dots and matrix, respectively.

The transformation of terms describing the potential energy is more complex. The full energy can be then presented as follows

$$E = T + V = \{ T^1 - \Delta T^1 \} + \{ T^0 + [-T^0 + \Delta T^0] \} + V^{00} +$$

$$+ V^{11} + [(-V^{00} + \delta V^{00}) + \Delta V^{11} + \Delta V^{10} + \Delta V^{01}]. \quad (3)$$

In relations (2), (3) the energy of crystal containing a QD is presented as a sum of energies of two (virtual) crystals and interaction energy between their vibrations. It should be noted that according to Eqs.(2), (3) the terms T^{00} and V^{00} are really excluded from general expression (3) but we conserve them to make the following consideration more consistent.

2.2 Secondary quantization and Hamiltonian of crystal

It is convenient to make the following analysis by using the secondary quantization procedure.

Hamiltonian of crystal can be obtained from the formulae for energy, Eqs.(2, 3), by expression of values $u_{n\alpha}^k$ by creation-annihilation phonon operators, $b_{q,s}^+$, $b_{q,s}$, of branch s and wave vector q. Shifts of atoms and their velocities are real values $u_{n,\alpha}^k = u_{n,\alpha}^{*k}$, $\dot{u}_{n,\alpha}^k = \dot{u}_{n,\alpha}^{*k}$ and the corresponding operators are hermitian and equal

$$u_{n,\alpha}^{j,k} = \frac{1}{\sqrt{\tilde{N}}} \sum_{q,s} A_{s,\alpha}^{j,k}(q) \exp(iqn) \varphi_{q,s},$$

$$\dot{u}_{n,\alpha}^{j,k} = \frac{i}{\sqrt{\tilde{N}}} \sum_{q,s} A_{s,\alpha}^{j,k}(q) \omega_{q,s} \exp(iqn) \pi_{-q,s}, \qquad (4)$$

$$\varphi_{q,s} = \frac{1}{\sqrt{2}} (b_{q,s} + b_{-q,s}^+) = \varphi_{-q,s}^+,$$

$$\pi_{q,s} = \frac{1}{\sqrt{2}} (b_{q,s}^+ - b_{-q,s}) = -\pi_{-q,s}^+,$$

$$[\varphi_{q,s}, \pi_{q',s'}] = \delta_{q,q'} \delta_{s,s'}, \qquad (5a)$$

$$A_{s,\alpha}^{j,k}(q) = \sqrt{\frac{\hbar}{M \omega_{q,s}}} e_{s,\alpha}^{j,k}(q), \quad e_{s,\alpha}^{*j,k}(q) = e_{s,\alpha}^{j,k}(-q) \qquad (5b)$$

where $e_{s,\alpha}^{j,k}(q)$ and M are amplitude of vibration and mass of atoms in unit cells respectively. We also will number the phonon branches by indexes s_0, s_1 for QD and matrix respectively.

In Eqs.(4a-c) the wave vector q is changed in the broad region $-\pi / a \leq q \leq \pi / a$, where a is a lattice constant of initial lattice. For new great unit cell the lattice constant is $a_L = La$, therefore the wave vector is changed in some other limits, $-\pi / La \leq \tilde{q} \leq \pi / La$, and both wave vectors are connected by relation

$$q = b_g + \tilde{q}, \quad b_g = bg, \quad b = \frac{2\pi}{La}, \quad -\frac{L}{2} \leq g \leq \frac{L}{2},$$

$$g = 0, \pm 1, \pm 2, \dots, \qquad (6)$$

where b is a new reciprocal lattice vector and the cyclic Born-Karman conditions for crystal with QD are the same: $\exp(ib_x N_x) = \exp[i(2\pi / La)(NaL)] = \exp(i2\pi N) = 1$.

Hamiltonian of crystal with QD in the secondary quantization representation is given by group of Eqs. (7)

$$H = \sum_{\widetilde{q},g,s_1} \omega_{\widetilde{q}+g,s_1} b^+_{\widetilde{q}+g,s_1} b_{\widetilde{q}+g,s_1} + \sum_{\widetilde{q},g,s_0} \omega_{\widetilde{q}+g,s_0} b^+_{\widetilde{q}+g,s_0} b_{\widetilde{q}+g,s_0} -$$

$$-\frac{1}{2}\sum_{\widetilde{q},g,s_0,g',s_0'}[T^{(0)}_{\widetilde{q}}({}^{s_0,s_0'}_{g,g'})\delta_{g,g'} - \Delta T^{(0)}_{\widetilde{q}}({}^{s_0,s_0'}_{g,g'})a^{L_0}_{(g'-g)}]\cdot$$

$$\cdot \pi_{-(g+\widetilde{q}),s_0}\pi^+_{-(g'+\widetilde{q},s_0')} -$$

$$-\frac{1}{2}\sum_{\widetilde{q},g,s_1,g',s_1'}\Delta T^{(1)}_{\widetilde{q}}({}^{s_1,s_1'}_{g,g'})a^{L_0}_{(g'-g)}\pi_{-(g+\widetilde{q}),s_1}\pi^+_{-(g'+\widetilde{q},s_1')} -$$

$$-\frac{1}{2}\sum_{\widetilde{q},g,s_0,g',s_0'}[\delta_{g,g'}L\overline{V}_{\widetilde{q}}({}^{s_0,s_0'}_{g,g'}) - a^{L_0}_{g+\widetilde{q}}a^{*L_0}_{g'+\widetilde{q}}LV_{\widetilde{q}}({}^{s_0,s_0'}_{g,g'})]\cdot$$

$$\cdot \varphi_{g+\widetilde{q},s_0}\varphi^+_{g'+\widetilde{q},s_0'} -$$

$$-\frac{1}{2}\sum_{\widetilde{q},g,s_1,g',s_1'}[(a^L_{g+\widetilde{q}}-a^{L_0}_{g+\widetilde{q}})a^{*L_0}_{g'+\widetilde{q}} + a^{L_0}_{g+\widetilde{q}}(a^{*L}_{g'+\widetilde{q}}-a^{*L_0}_{g'+\widetilde{q}})+$$

$$+a^{L_0}_{g+\widetilde{q}}a^{*L_0}_{g'+\widetilde{q}}]LV_{\widetilde{q}}({}^{s_1,s_1'}_{g,g'})\varphi_{g+\widetilde{q},s_1}\varphi^+_{g'+\widetilde{q},s_1'} +$$

$$+\frac{1}{2}\sum_{\widetilde{q},g,s_1,g',s_1'}(a^L_{g+\widetilde{q}}-a^{L_0}_{g+\widetilde{q}})a^{*L_0}_{g'+\widetilde{q}}LV_{\widetilde{q}}({}^{s_1,s_0'}_{g,g'})\varphi_{g+\widetilde{q},s_1}\varphi^+_{g'+\widetilde{q},s_0'} +$$

$$+\frac{1}{2}\sum_{\widetilde{q},g,s_1,g',s_1'}a^{L_0}_{g+\widetilde{q}}(a^{*L}_{g'+\widetilde{q}}-a^{*L_0}_{g'+\widetilde{q}})LV_{\widetilde{q}}({}^{s_0,s_1'}_{g,g'})\varphi_{g+\widetilde{q},s_0}\varphi^+_{g'+\widetilde{q},s_1'}.$$

$$a^{L_0}_{g+\widetilde{q}} = \frac{L_0}{L}f^{L_0}_{g+\widetilde{q}}, \quad a^L_{g+\widetilde{q}} = f^L_{g+\widetilde{q}}, \tag{7}$$

$$f^{L_0}_{g+\widetilde{q}} = \frac{1}{L_0}\sum_{n_0}\exp[i(\widetilde{q}+b_g)n_0] \tag{8}$$

It is seen from Hamiltonian that wave vector $-\pi/La \leq \widetilde{q} \leq \pi/La$ is conserved in this quantum structure.

2.3 Equations for Green functions

Intensity of light scattering is expressed by Fourier component of retarded Green function (GF) on the phonon operators $\varphi_{g+\widetilde{q},s}$ (we will use the operators $\varphi_{p+k,\alpha}$ where $\alpha = \{\alpha_0,\alpha_1\}$ characterizes the phonon branch of both the QD and the matrix one). The GF is given by expression

$$<< \varphi_{p+k,\alpha}(t);\varphi^+_{p'+k',\alpha}(0) >>$$

$$= -i\Theta(t) < [\varphi_{p+k,\alpha}(t);\varphi^+_{p'+k',\alpha'}(0)] >, \tag{9}$$

$\Theta(t)$ is a step function; $[a, b]$ is a commutator of two operators; $<....>$ statistical average of operators;

$$\varphi_{p+k,\alpha}(t) = \exp(iHt)\varphi_{p+k,\alpha}\exp(-iHt)$$

System of equations for Green functions is following

$$i\frac{\partial}{\partial t} << \varphi_{p+k,\alpha_0}(t);\varphi^+_{p'+k',\alpha'}(0) >>=$$

$$<< i\frac{\partial}{\partial t}\varphi_{p+k,\alpha_0}(t);\varphi^+_{p'+k',\alpha'}(0) >> =$$

$$=\sum_{s_0}[-\delta_{s_0,\alpha_0}\omega_{p+k,\alpha_0} + \Delta T^{(0)}_k({}^{s_0,\alpha_0}_{p,p})(1-a^{L_0}_0)]\cdot$$

$$\cdot << \pi_{-(p+k),s_0}\varphi^+_{p'+k',\alpha'} >> \tag{10a}$$

$$i\frac{\partial}{\partial t} << \pi_{-(p+k),s}(t);\varphi^+_{p'+k',\alpha'}(0) >>=$$

$$-\delta(t)\delta_{s,\alpha'}\delta_{p+k,p'+k'}$$

$$-\omega_{p+k,s} << \varphi_{p+k,s}(t);\varphi^+_{p'+k',\alpha'}(0) >> -$$

$$-2\sum_{g_1,\beta}\widetilde{V}_k({}^{\beta,s}_{g_1,p}) << \varphi_{g_1+k,\beta}(t);\varphi^+_{p'+k',\alpha'}(0) >>, \tag{10b}$$

After Fourier transformation and inserting (10b) into (10a) we obtain the following system

$$\omega^2 << \varphi_{p+k,\alpha_0}(t);\varphi^+_{p'+k',\alpha'}(0) >>_\omega=$$

$$\omega_{p+k,\alpha_0}a^{L_0}_0\delta_{\alpha_0,\alpha'}\delta_{p+k,p'+k'} + (-\omega_{p+k,\alpha_0}a^{L_0}_0) + \{-$$

$$\sum_{g_1,\beta_0}a^{L_0}_{g_1+k}a^{*L_0}_{p+k}LV_k({}^{\beta_0,\alpha_0}_{g_1,p}) << \varphi_{g_1+k,\beta_0}(t);\varphi^+_{p'+k',\alpha'}(0) >>_\omega -$$

$$-\sum_{g_1,\beta_1}(a^L_{g_1+k}-a^{L_0}_{g_1+k})a^{*L_0}_{p+k}LV_k({}^{\beta_1,\alpha_0}_{g_1,p})\cdot$$

$$\cdot << \varphi_{g_1+k,\beta_1}(t);\varphi^+_{p'+k',\alpha'}(0) >>_\omega\}, \tag{11}$$

$$[\omega^2 - \omega^2_{p+k,\alpha_1}(1-a^{L_0}_0)] << \varphi_{p+k,\alpha_1}(t);\varphi^+_{p'+k',\alpha'}(0) >>_\omega=$$

$$\omega_{p+k,\alpha_1}(1-a^{L_0}_0)\delta_{\alpha_1,\alpha'}\delta_{p+k,p'+k'} - [\omega_{p+k,\alpha_1}(1-a^{L_0}_0)]\cdot$$

$$\cdot\{\sum_{g_1,\beta_1}[(a^L_{g_1+k}-a^{L_0}_{g_1+k})a^{*L_0}_{p+k} + a^{L_0}_{g_1+k}a^{*L}_{p+k}]LV_k({}^{\beta_1,\alpha_1}_{g_1,p})\cdot$$

$$\cdot << \varphi_{g_1+k,\beta_1}(t);\varphi^+_{p'+k',\alpha'}(0) >>_\omega -$$

$$-\sum_{g_1,\beta_0}a^{L_0}_{g_1+k}(a^{*L}_{p+k}-a^{*L_0}_{p+k})LV_k({}^{\beta_0,s_1}_{g_1,p})\cdot$$

$$\cdot << \varphi_{g_1+k,\beta_0}(t);\varphi^+_{p'+k',\alpha'}(0) >>_\omega\} \tag{12}$$

For simplicity we will consider the case when both (virtual) crystals consisting of the QD and the matrix material have only one (optical or acoustical) longitudinal vibration; that means $\alpha_0 = \beta_0$, $\alpha_1 = \beta_1$ and summation on β_0 and β_1 disappears in Eq.(11, 12). Beside let us suppose that constants characterizing the interaction between vibrations is independent on the wave vector, i.e. $LV_k({}^{\alpha,\beta}_{g,p}) = V^{\alpha,\beta}$ and introduce the

$$f^{L_0,L_0}_{\alpha_0}(\omega,k) = \sum_p \frac{a^{L_0}_{p+k}a^{*L_0}_{p+k}\widetilde{\omega}_{p+k,\alpha_0}}{\Delta(\omega,p+k,\alpha_0)},$$

$$f^{L-L_0,L_0}_{\alpha_0}(\omega,k) = \sum_p \frac{(a^L_{p+k}-a^{L_0}_{p+k})a^{*L_0}_{p+k}\widetilde{\omega}_{p+k,\alpha_0}}{\Delta(\omega,p+k,\alpha_0)}, \tag{13}$$

The relations (11) and (12) give rise to the expressions for Fourier components of Green functions expressed by crystal parameters and frequency. The corresponding relations can be written as

$$<< \varphi_{p+k,\alpha_0}(t);\varphi^+_{p'+k',\alpha'}(0) >>_\omega=$$

$$=\frac{1}{\Delta(\omega,p+k,\alpha_0)}\{\widetilde{\omega}_{p+k,\alpha_0}\delta_{\alpha_0,\alpha'}\delta_{p,p'}\delta_{k,k'}+$$

$$+\widetilde{\omega}_{p+k,\alpha_0}a^{*L_0}_{p+k}[V^{\alpha_0\alpha_0}\frac{1}{\Delta(\omega,k)}\cdot$$

$$\cdot\frac{a^{L_0}_{p'+k'}\widetilde{\omega}_{p'+k',\alpha_0}}{\Delta(\omega,p'+k',\alpha_0)}\delta_{\alpha_0,\alpha'}\delta_{k,k'}+$$

$$+V^{\alpha_1\alpha_0}\frac{1}{\Delta(\omega,k)}\frac{(a^L_{p'+k'}-a^{L_0}_{p'+k'})\widetilde{\omega}_{p'+k',\alpha_1}}{\Delta(\omega,p'+k',\alpha_1)}\delta_{\alpha_1,\alpha'}\delta_{k,k'}]\}$$

$$(14a)$$

$$<<\varphi_{p+k,\alpha_1}(t);\varphi^+_{p'+k',\alpha'}(0)>>_\omega=$$

$$\frac{1}{\Delta(\omega,p+k,\alpha_1)}\{\widetilde{\omega}_{p+k,\alpha_1}\delta_{\alpha_1,\alpha'}\delta_{p,p'}\delta_{k,k'}-$$

$$-\widetilde{\omega}_{p+k,\alpha_1}[V^{\alpha_1\alpha_1}(a^{*L_0}_{p+k}\frac{1}{\Delta(\omega,k)}\cdot$$

$$\cdot\frac{(a^L_{p'+k'}-a^{L_0}_{p'+k'})\widetilde{\omega}_{p'+k',\alpha_1}}{\Delta(\omega,p'+k',\alpha_1)}\delta_{\alpha_1,\alpha'}\delta_{k,k'}+$$

$$+a^{*L}_{p+k}\frac{1}{\Delta(\omega,k)}\frac{a^{L_0}_{p'+k'}\widetilde{\omega}_{p'+k',\alpha_1}}{\Delta(\omega,p'+k',\alpha_1)}\delta_{\alpha_1,\alpha'}\delta_{k,k'})-$$

$$-(a^{*L}_{p+k}-a^{*L_0}_{p+k})V^{\alpha_0\alpha_1}\frac{1}{\Delta(\omega,k)}\cdot$$

$$\cdot\frac{a^{L_0}_{p'+k'}\widetilde{\omega}_{p'+k',\alpha_0}}{\Delta(\omega,p'+k',\alpha_0)}\delta_{\alpha_0,\alpha'}\delta_{k,k'}]\}$$

$$(14b)$$

3 Intensity of light Raman scattering

We will consider that only one longitudinal branch for each crystal there is α_0 and α_1

To simplify the formulae for Raman scattering intensity we will neglect the dependence on wave vector in the tensor of susceptibility, supposing $\widetilde{\chi}^{s_j}_{k',\lambda',k,\lambda}(b_g+Q)=\widetilde{\chi}^{s_j}_{k',\lambda',k,\lambda}$. Then intensity of Raman scattering can be described by expression

$$I_{p',\lambda',p,\lambda}(\omega)\sim-[1+n(\omega)]\cdot$$

$$\cdot\mathrm{Im}\{I^{00}_{p',\lambda',p,\lambda}+I^{01}_{p',\lambda',p,\lambda}+I^{10}_{p',\lambda',p,\lambda}+I^{11}_{p',\lambda',p,\lambda}\},\qquad(15)$$

where

$$I^{00}_{p',\lambda',p,\lambda}=\widetilde{\chi}^{\alpha_0}_{k',\lambda',k,\lambda}\widetilde{\chi}^{*\alpha_0}_{k',\lambda',k,\lambda}\{f^{L_0,L_0}_{\alpha_0}(\omega,Q)+$$

$$+\frac{V^{\alpha_0,\alpha_0}}{\Delta(\omega,Q)}f^{L_0,L_0}_{\alpha_0}(\omega,Q)f^{L_0,L_0}_{\alpha_0}(\omega,Q)\},\qquad(16a)$$

$$I^{01}_{p',\lambda',p,\lambda}=\widetilde{\chi}^{\alpha_0}_{k',\lambda',k,\lambda}\widetilde{\chi}^{*\alpha_1}_{k',\lambda',k,\lambda}\frac{V^{\alpha_1,\alpha_0}}{\Delta(\omega,Q)}f^{L_0,L_0}_{\alpha_0}(\omega,Q)\cdot$$

$$\cdot\{\frac{(a^L_Q-a^{L_0}_Q)\widetilde{\omega}_{\alpha_1,Q}}{\Delta(\omega,Q,\alpha_1)}-f^{L-L_0,L_0}_{\alpha_1}(\omega,Q)\},\qquad(16b)$$

$$I^{10}_{p',\lambda',p,\lambda}=\widetilde{\chi}^{\alpha_1}_{k',\lambda',k,\lambda}\widetilde{\chi}^{*\alpha_0}_{k',\lambda',k,\lambda}\frac{V^{\alpha_0,\alpha_1}}{\Delta(\omega,Q)}f^{L_0,L_0}_{\alpha_0}(\omega,Q)\cdot$$

$$\cdot\{\frac{(a^{\circ L}_Q-a^{*L_0}_Q)\widetilde{\omega}_{\alpha_1,Q}}{\Delta(\omega,Q,\alpha_1)}-f^{L_0,L-L_0}_{\alpha_1}(\omega,Q)\},\qquad(16c)$$

$$I^{11}_{p',\lambda',p,\lambda}=\widetilde{\chi}^{\alpha_1}_{k',\lambda',k,\lambda}\widetilde{\chi}^{*\alpha_1}_{k',\lambda',k,\lambda}\cdot$$

$$\cdot(\frac{[1-a^{L_0}_0-a^{*L_0}_0]\widetilde{\omega}_{\alpha_1,Q}}{\Delta(\omega,Q,\alpha_1)}+f^{L_0,L_0}_{\alpha_1}(\omega,Q)-$$

$$-\frac{V^{\alpha_1,\alpha_1}}{\Delta(\omega,Q)}\{\frac{\widetilde{\omega}_{\alpha_1,Q}}{\Delta(\omega,Q,\alpha_1)}\cdot$$

$$\cdot[a^{*L_0}_Q(\frac{(a^L_Q-a^{L_0}_Q)\widetilde{\omega}_{\alpha_1,Q}}{\Delta(\omega,Q,\alpha_1)}-f^{L-L_0,L_0}_{\alpha_1}(\omega,Q))+$$

$$+a^{*L}_Q(\frac{a^{L_0}_Q\widetilde{\omega}_{\alpha_1,Q}}{\Delta(\omega,Q,\alpha_1)}-f^{L_0,L_0}_{\alpha_1}(\omega,Q))]-$$

$$-[f^{L_0,L_0}_{\alpha_1}(\frac{(a^L_Q-a^{L_0}_Q)\widetilde{\omega}_{\alpha_1,Q}}{\Delta(\omega,Q,\alpha_1)}-f^{L-L_0,L_0}_{\alpha_1}(\omega,Q))+$$

$$+f^{L_0,L}_{\alpha_1}(\frac{a^{L_0}_Q\widetilde{\omega}_{\alpha_1,Q}}{\Delta(\omega,Q,\alpha_1)}-f^{L_0,L_0}_{\alpha_1}(\omega,Q))]\}).\qquad(16d)$$

$$\Delta(\omega,k)=[1-f^{L_0L_0}_{\alpha_0}(\omega,k)V^{\alpha_0\alpha_0}+f^{L-L_0,L_0}_{\alpha_1}(\omega,k)$$

$$V^{\alpha_1\alpha_1}+f^{L_0,L}_{\alpha_1}(\omega,k)V^{\alpha_1\alpha_1}],\qquad(17)$$

a). If constants of interaction V^{α_0,α_0}, V^{α_0,α_1}, V^{α_1,α_1}, between phonon branches are small the Eq.(17) reduces to more simple one because intensity is described in this case by two following terms

$$I^{00}_{p',\lambda',p,\lambda}+I^{11}_{p',\lambda',p,\lambda}=$$

$$=\widetilde{\chi}^{\alpha_0}_{k',\lambda',k,\lambda}\widetilde{\chi}^{*\alpha_0}_{k',\lambda',k,\lambda}f^{L_0,L_0}_{\alpha_0}(\omega,Q)+\widetilde{\chi}^{\alpha_1}_{k',\lambda',k,\lambda}\widetilde{\chi}^{*\alpha_1}_{k',\lambda',k,\lambda}$$

$$[\frac{(1-a^{L_0}_0-a^{*L_0}_0)\widetilde{\omega}_{\alpha_1,Q}}{\Delta(\omega,Q,\alpha_1)}+f^{L_0,L_0}_{\alpha_1}(\omega,Q)].\qquad(18a)$$

It is important to note that obtained expressions for intensity of light scattering are permitted for description of processes both with participation of the optical phonons and the acoustical ones. Details of scattering depend on the character of dispersion of phonon branches, $\omega_{\alpha_j,Q}$.

4 Numerical model calculations.

The fulfilled numerical calculations showed a qualitative correlation with the experimental results. As an example in Fig. 2 are shown our experimental and calculated Raman spectra for a five-layer Si/GeSi QD structure. In the calculation a common sinusoidal dispersion law was used for the acoustical phonon branch. This may be one of the reasons for the observed deviation of the calculated spectrum from the experimental one. Another important factor that can affect the shape of the theoretical spectrum

can be a more correct choice of the constant describing interaction between vibrations in Eqs.16,17.
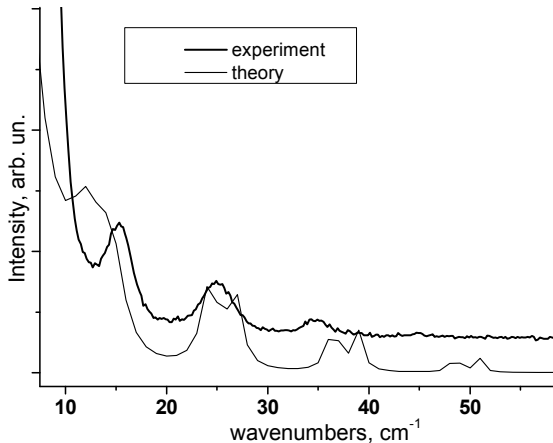

Fig. 2. Comparison of the experimental and calculated Raman spectra for a five-layer Si/GeSi QD structure.

5 Conclusions

A theoretical investigation of the phonon spectrum of crystal structures with quantum dots was performed taking into account the real crystal structure of both the quantum dots and surrounding matrix. The numerically calculated spectrum shows a qualitative correlation to the experimental Raman spectrum of a multilayer Ge/Si QD structure.

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