18th Int. Symp. “Nanostructures: Physics and Technology”
St Petersburg, Russia, June 21–26, 2010

Intervalley scattering of electrons by confined and interface optical phonons in $(GaAs)_m(AlAs)_n$ (001) superlattices

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Abstract. Intervalley $\Gamma - M$ and $\Gamma - \Sigma$ transitions inside the conduction bands of superlattices $(GaAs)_m(AlAs)_n$ (001) caused by the optical lattice vibrations are investigated by a pseudopotential method and a phenomenological model of the interatomic bonding forces. The analysis of quantum-size effects to the electrons' and phonons' states is carried out, the interpretation of dependences of the deformation potentials versus a thickness of layers in the superlattices is given. It is shown that the intensity of intervalley scattering became maximal when the electrons' and phonon's states are both localized at the same layers of a superlattice. The interface vibrations appear in the superlattices with the layers thick enough $(m, n \geq 4)$. They invoke a rather weak electronic transitions inside the higher conduction bands.

Due to multivalley character of conduction bands, mixed character of lattice vibrations and a favorable combination of phonon's and electrons' spectra parameters, a superlattice $(GaAs)_m(AlAs)_n(001)$ is of a great interest for a research and for the technical use of effects produced by the intervalley scattering of electrons by short-wave phonons. This scattering plays the important role in optical and transport properties of nanostructures, in particular, it results in leakage currents in cascade lasers, in a decrease of electrons' mobility inside the channels of transistors, in the occurrence of peculiarities in the hot photoluminescence spectra etc. [1,2]. Owing to the size quantization the electron-phonon interaction in superlattices has a complex character and it is described by the large number of deformation potentials for multiple scattering channels. The most intensive channels of scattering in superlattices are the analogues of $\underline{X} - \underline{X}$ transitions in GaAs, AlAs (hereafter the sphalerite's states are underlined). They involve optical vibrations confined inside layers or phonons localized near a heteroboundary.

In the present work the influence of confined and interface optical vibrations to the processes of the intervalley scattering in superlattices $(GaAs)_m(AlAs)_n(001)$ (m,n = 1,...,8) with the thin layers is investigated on the basis of the microscopic description of electron and phonon states.

The intensity of electron intervalley scattering from an initial state $\mu\mathbf{k}$ to the final state $\mu\prime\mathbf{k}\prime$ ($\mu, \mathbf{k}$ label the band number and the wave vector) is determined by a deformation potential according to [3]:

$$\left|D^s_{\mu\mathbf{k},\mu\prime\mathbf{k}\prime}\right| = \left|\sum_{i,\alpha}\left(\frac{M}{m_\alpha}\right)^{1/2}\left(e^\alpha_i(s,\mathbf{q})\cdot d^\alpha_i(\mu\mathbf{k},\mu\prime\mathbf{k}\prime)\right)\right|$$

where m_α and M are masses of $\alpha - th$ ion and the unit cell as a whole correspondingly, $\mathbf{e}^\alpha(s,\mathbf{q})$ is a phonon polarization vector (s - labels a phonon branch), d^α_i is a matrix element between the functions of initial and final states of a gradient of the atom potential, $\mathbf{q} = \mathbf{k}\prime - \mathbf{k}$ is the phonon wave vector. The electron states in superlattices are calculated by a method of pseudopotential [4]. The behavior of the conduction band levels for superlattices with even monolayers numbers m and n is shown at fig.1. The behavior of superlattice's levels correlates with those in the corresponding virtual crystals (VC). The tetragonal component of superlattice's potential results in lowering of electronic levels relative to VC levels. The greatest shifts take place for $\Gamma_1^{(1)}$, Γ_3 and M_5 conduction states located inside the $\underline{\Gamma}$ and $\underline{X}$ quantum wells. The M_1, M_4 and $\Gamma_1^{(2)}$ conduction states, being localized at anions, are shifted in much less extent.

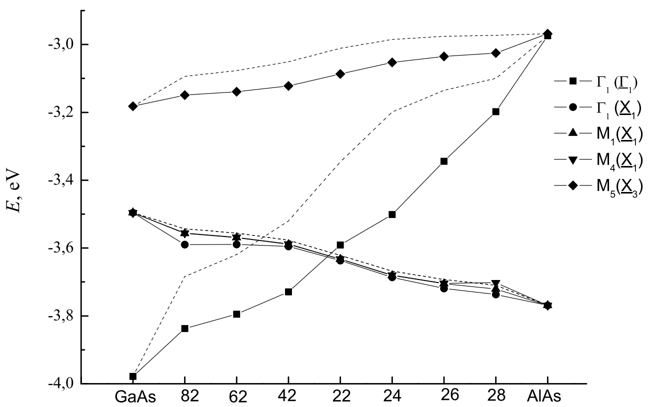

Fig. 1. Levels of a conduction band of superlattices (solid lines and symbols) for Γ, M states and solid solutions (dashed lines) for $\underline{\Gamma}, \underline{X}$ states in an absolute scale of energy. The figures indicate quantities of monolayers m, n.

The phonon spectra of superlattices were calculated with a phenomenological model of the bonding forces in the mass-defect approach [5].The optical branches at high frequencies $\sim 10 - 12$ THz are connected with vibrations of Al atoms. They are separated from other branches by a gap. Optical vibrations which frequencies, lying in the frequency interval of a binary component, are localized inside the corresponding layers of a superlattice.Phonons with symmetry M_5 are located in AlAs layers of a superlattice $(GaAs)_8(AlAs)_2$. They are located in GaAs layers of $(GaAs)_2(AlAs)_8$ (fig.2). These vibrations have a mixed LO-TO character. When thickness of layers in superlattices is large $(m, n \geq 4)$ then the interface optical phonons ($\mathbf{q} \perp z$) appear in the "cavities" between acoustic and optical branches of phonon's spectrum which involves the vibration of cations near to a heteroboundary. The modules of polarization vectors $\mathbf{e}^{\alpha}(s, \mathbf{q}_{\Sigma})$ for the interface TO-type phonon ($\omega(\mathbf{q}_{\Sigma})$=7,40 THz) in a superlattice $(GaAs)_6(AlAs)_4$ and the interface LO type phonon ($\omega(\mathbf{q}_{\Sigma})$=11,075 THz) in a superlattice $(GaAs)_4(AlAs)_6$ are shown at fig.3. In the mass-defect approach the interface phonons appear at a wave vector in a middle point of Σ line: $\mathbf{q}_{\Sigma} = (\pi/a_0, 0, 0)$. Note, that other type of interface phonons were found at the edge of a zone Brillouine beyond the bounds of mass-defect approximation taking into account the differences of second-neighbors Ga-Al force constants from those of Ga-Ga and Al-Al [6]. These phonons of TO-type involve the vibrations of atoms Ga along [011] direction mostly, phonons of LO type involve vibrations of atoms Al in a direction [211]. Displacements in TO- type phonons are more localized near to the border due to the greater value of the imaginary part of a phonon wave vector [7].

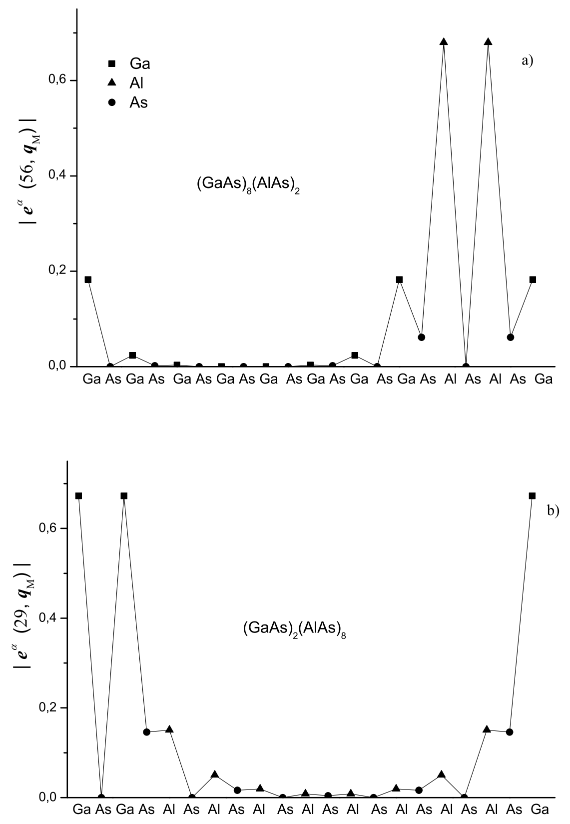

Fig. 2. Module of M_5 - phonon polarization vector $|\mathbf{e}^{\alpha}(s, \mathbf{q})|$: a) of a branch with number s = 56 and frequency ω = 9,700 THz of a superlattice $(GaAs)_8(AlAs)_2$, b) of a branch with number s = 29 and frequency ω = 6,820 THz of a superlattice $(GaAs)_2(AlAs)_8$.

The calculated deformation potentials for the transitions between Γ and M conduction band valleys in superlattices with a participation of phonons, confined inside the layers, are given in tab.1. The outline of bands and of the intervalley transitions are shown at fig.4. In superlattices with only one AlAs monolayer the scattering of electrons by vibrations of Al and Ga has approximately identical intensity due to a weak localization of wave functions of initial and final states in a narrow quantum X- well. The localization of electrons and phonons in AlAs layers enhances with a growth of a

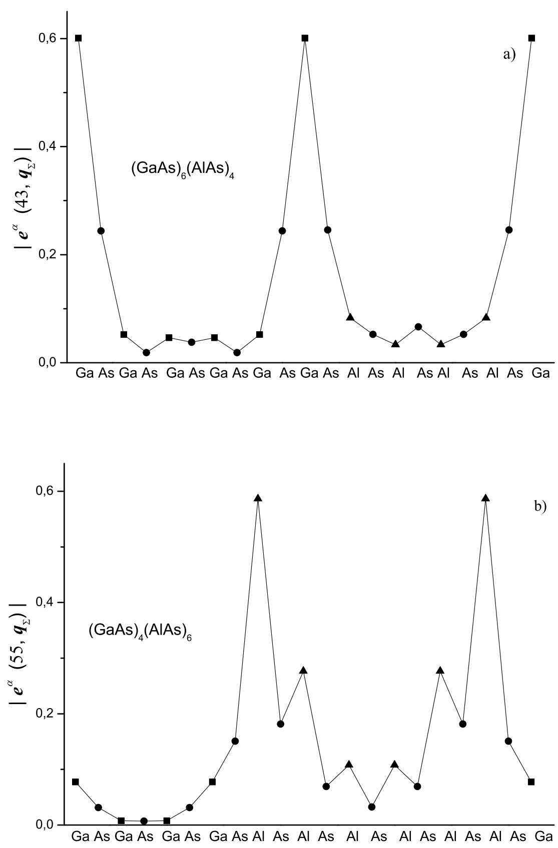

Fig. 3. Module of Σ_1-phonon polarization vector $|\mathbf{e}^{\alpha}(s, \mathbf{q})|$: a) of a branch with number s = 43 and frequency ω= 7,402 THz of a superlattice $(GaAs)_6(AlAs)_4$, b) of a branch with number s = 55 and frequency ω= 11,075 THz of a superlattice $(GaAs)_4(AlAs)_6$.

thickness of these layers. The vibrations of Al atoms begin to play the main role in $\Gamma - M$ scattering, the value of deformation potential became closer to the potential of $\underline{X} - \underline{X}$ scattering in AlAs.

Table 1. Deformation potentials $\left|D^s_{\mu\Gamma,\mu' M}\right|$ for Γ-M electron transitions in the conduction bands of superlattices $(GaAs)_m(AlAs)_n$ with thin AlAs layers. In brackets the frequencies (THz) are given of M phonons is specified. The bold font indicates the potentials due to the optical phonons confined in AlAs layers, other potentials relate to vibrations of Ga atoms.

Superlattice	$m = 9$ $n = 1$	$m = 8$ $n = 2$	$m = 7$ $n = 3$
Transition, energy, eV	$\Gamma_3 - M_5$ 0.014	$\Gamma_1^{(2)} - M_4$ 0.032	$\Gamma_3 - M_5$ 0.046
$\left|D^s_{\mu\Gamma,\mu' M},\right|$, $eV/\AA$	2.95(6.52) 4.07(6.78) **4.28**(10.61)	2.04(5.61) 1.46(6.26) 1.69(6.99) 1.05(7.50) **9.75**(9.70)	**5.30**(9.06) **7.98**(10.52) **4.71**(11.72)

Deformation potentials for $\Gamma - \Sigma$ transitions with the participation of interface and other phonons are given in tab.2. Phonons with low frequencies (4-5 THz) are accompanied by vibrations of atoms in both lattices. Interface phonons cause the intervalley transitions in the higher conduction

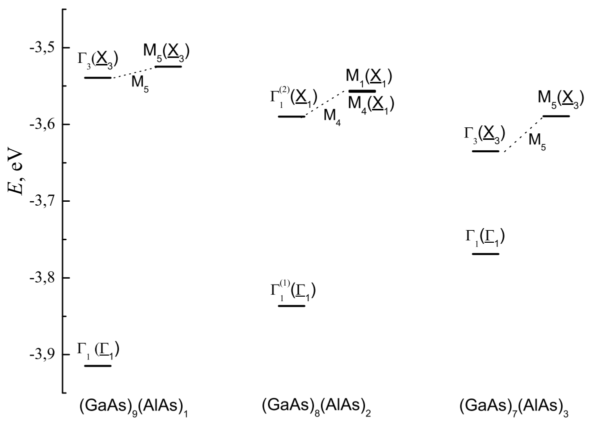

Fig. 4. Conduction band levels in superlattices with the thin AlAs layers (in the absolute energy scale). The VC states are specified in brackets. Dashed lines show the intervalley transitions with the participation of phonons confined in AlAs layers.

bands. In a $(GaAs)_6(AlAs)_4$ superlattice the interface vibrations have TO - type vibrations of Ga atoms, in other superlattices they correspond to the LO-type vibrations of Al atoms. All channels of the scattering have a comparable value of the intensity.

Table 2. Deformation potentials$\left|D^s_{\mu\Gamma,\mu' M}\right|$ for $\Gamma-\Sigma$ electron transitions in the conduction band of superlattices $(GaAs)_m(AlAs)_n$. In brackets the phonon frequencies are given in THz. The bold font indicates potentials due to the interface vibrations.

Superlattice	$m=6$ $n=4$	$m=8$ $n=8$	$m=4$ $n=6$
Transition, energy, eV	$\Gamma_1^{(2)}-\Sigma_2$ 1.56	$\Gamma_1^{(1)}-\Sigma_1$ 1.65	$\Gamma_1^{(1)}-\Sigma_1$ 1.67
	1.60(4.83)	1.54(8.89)	1.46(4.99)
	1.46(5.19)	1.02(10.65)	2.09(5.41)
	1.20(5.82)	**1.52**(11.07)	4.14(9.62)
$\left|D^s_{\mu\Gamma,\mu'\Sigma}\right|$, $eV/\AA$	1.04(6.95)		1.02(10.30)
	1.28(7.41)		1.73(10.63)
	2.77(9.16)		**1.90**(11.07)
	2.67(10.20)		2.45(11.56)
	2.91(11.09)		
	1.23(11.79)		

In a summary, in this work the deformation potentials are obtained for $\Gamma-M$ and $\Gamma-\Sigma$ intervalley transitions in a conduction band of superlattices $(GaAs)_m(AlAs)_n(001)$ with the participation of optical M-phonons confined inside the binary layers and optical Σ-phonons localized near the heteroboundary. Is shown that the intensity of $\Gamma-M$ transitions increases with a growth of a fraction of Al due to amplification of electronic density in quantum X wells. Interface phonons arise in superlattices with the layers thick enough. The $\Gamma-\Sigma$ transitions induced by them in the higher conduction bands have a rather weak intensity and are almost independent on a layers' thickness. The deformation potentials obtained here can be used for a modeling and interpretation of transport and optical properties of GaAs/AlAs (001) superlattices and heterostructures.

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