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Electronic States in Type-II Superlattices

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In this paper the electronic states in type-II superlattices are demonstrated. Band dispersions of InAs/GaSb periodic structure were calculated with the respect of the light and the heavy holes states mixing at InAs/GaSb interfaces. The effect of narrow energy band gap of InAs was taken into account and the wavelengths corresponding to optical transitions in the superlattice were presented.

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1. Introduction

The type-II superlattices are expected to be the important part of modern semiconductor devices. They may be used in the infrared radiation detectors or in the quantum cascade laser structures. Optical properties of a superlattice (SL) may be described if its band structure is known. This means that the band dispersions describing electrons and heavy and light holes should be found. One kind of the type-II superlattice is a periodic InAs/GaSb system. GaAs and InSb bonds are possible at the interfaces (IFs) of such a structure. Both of the bonds are foreign to InAs and GaSb — this causes the wave function mixing at the IFs. In the work the coupled Hamiltonian which describes heavy hole (HH) and light hole (LH) interacting states, is considered [1]. The strength of the interaction is expressed by the dimensionless parameter t. Furthermore, because of the narrow energy band gap of InAs the influence of the valence band (VB) on the conduction band (CB) was taken into account. It was done with the help of the three-band Kane model in which LH states are coupled to the CB states throughout Kane's momentum matrix element π [2].

2. Method

The one-dimensional, periodic potential of the SL is shown in Fig. 1. Materials A (InAs) and B (GaSb) with the thickness $2a$ and $2b$, denote the barrier and the well in the VB (Fig. 1a), and, respectively, the well and the barrier in the CB (Fig. 1b).

HH and LH interacting states, are described by Schrödinger equation in the form [1]:

$$\begin{pmatrix} -\frac{\hbar^2}{2m_{\mathrm{H}}}\frac{\mathrm{d}^2}{\mathrm{d}z^2}+V(z) & \mathrm{i}T\left[\delta\left(z-b\right)-\delta\left(z+b\right)\right] \\ -\mathrm{i}T\left[\delta\left(z-b\right)-\delta\left(z+b\right)\right] & -\frac{\hbar^2}{2m_{\mathrm{L}}}\frac{\mathrm{d}^2}{\mathrm{d}z^2}+V(z) \end{pmatrix}\begin{pmatrix} \Psi_{\mathrm{H}}(z) \\ \Psi_{\mathrm{L}}(z) \end{pmatrix}=E\begin{pmatrix} \Psi_{\mathrm{H}}(z) \\ \Psi_{\mathrm{L}}(z) \end{pmatrix}, \tag{1}$$

where m_{H}, m_{L} are heavy hole and light hole masses. Both particles are described by the two-component envelope function formed by $\Psi_{\mathrm{H}}(z)$ and $\Psi_{\mathrm{L}}(z)$. The expressions $\pm\mathrm{i}T[\delta(z-b)-\delta(z+b)]$ with δ-function describe the interaction of HH and LH states at InAs/GaSb IFs determined by $T=t(625\ \mathrm{meV\ \AA})$.

Energies E, as eigenvalues defined by Eq. (1) describe HH and LH for $E=E_{\mathrm{HH}}$ and $E=E_{\mathrm{LH}}$, respectively.

Away from the IFs, $\Psi_{\mathrm{H}}(z)$ and $\Psi_{\mathrm{L}}(z)$ may be written as a sum of plane waves which propagate in the positive and in the negative z direction [1]:

$$\Psi_{\mathrm{H}}(z)=\begin{cases} c_{1\mathrm{H}}^{A}\,\mathrm{e}^{\mathrm{i}k_{\mathrm{H}}^{A}z}+c_{2\mathrm{H}}^{A}\,\mathrm{e}^{-\mathrm{i}k_{\mathrm{H}}^{A}z} \\ c_{1\mathrm{H}}^{B}\,\mathrm{e}^{\mathrm{i}k_{\mathrm{H}}^{B}z}+c_{2\mathrm{H}}^{B}\,\mathrm{e}^{-\mathrm{i}k_{\mathrm{H}}^{B}z} \end{cases},\quad \Psi_{\mathrm{L}}(z)=\begin{cases} c_{1\mathrm{L}}^{A}\,\mathrm{e}^{\mathrm{i}k_{\mathrm{L}}^{A}z}+c_{2\mathrm{L}}^{A}\,\mathrm{e}^{-\mathrm{i}k_{\mathrm{L}}^{A}z} & b\le z<b+2a \\ c_{1\mathrm{L}}^{B}\,\mathrm{e}^{\mathrm{i}k_{\mathrm{L}}^{B}z}+c_{2\mathrm{L}}^{B}\,\mathrm{e}^{-\mathrm{i}k_{\mathrm{L}}^{B}z} & -b\le z<b \end{cases}, \tag{2}$$

where $k_{\mathrm{H,L}}^{A} = \sqrt{2m_{\mathrm{H,L}}(E-V_0)/\hbar^2}$ and $k_{\mathrm{H,L}}^{B} =$

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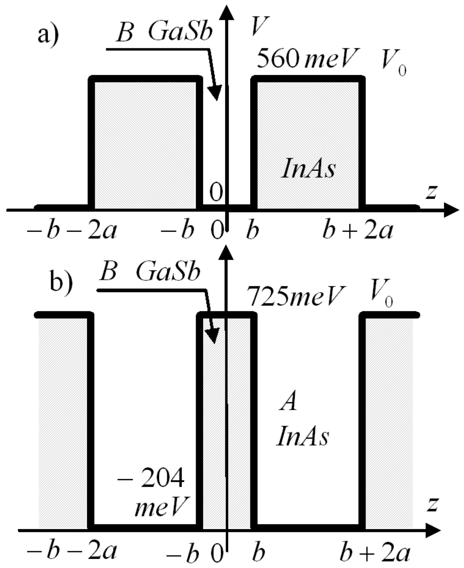

Fig. 1. The models of the potential energies $V(z)$ which describe (a) the VB and (b) the CB in InAs/GaSb superlattice. Parameters of the models are marked in the figures.

$\sqrt{2m_{\mathrm{H,L}}E/\hbar^2}$. The high of the potential barrier V_0 is marked in Fig. 1.

Simultaneously, $\Psi_{\mathrm{H}}(z)$ and $\Psi_{\mathrm{L}}(z)$ should fulfill the boundary conditions which concern their continuity at InAs/GaSb IFs and the Bloch periodicity throughout the SL. Boundary should conditions also ensure the continuity of the total flux of the particles across the IFs. These conditions lead to the 4×4 matrix for which the secular equation may be written in the form [1]:

$$\left(F_{\mathrm{H}}G_{\mathrm{L}} - t_{\mathrm{H}}^2\right)\left(F_{\mathrm{L}}G_{\mathrm{H}} - t_{\mathrm{L}}^2\right) - F_{\mathrm{H}}G_{\mathrm{H}}\delta L^2 - F_{\mathrm{L}}G_{\mathrm{L}}\delta H^2 + \delta H^2\delta L^2 + 2t_{\mathrm{H}}t_{\mathrm{L}}\delta H\delta L = 0. \quad (3)$$

The left side of Eq. (3) depends on $k_{\mathrm{H,L}}^A$, $k_{\mathrm{H,L}}^B$, $m_{\mathrm{H,L}}$, a, b, d, T, q, where $d = 2a+2b$ is the period of the SL and q is the wave vector which spans Brillouin zone (BZ) in the interval $\langle -\pi/d, \pi/d\rangle$. Because of the limited place in this article and because of large expressions which describe F_{H}, F_{L}, G_{H}, G_{L}, t_{H}, t_{L}, δH, δL we refer for details of the expressions to the work [1].

Dissolving of Eq. (3) in a given energy interval results in the requested band dispersions: $E_{\mathrm{HH}}(q)$, $E_{\mathrm{LH}}(q)$.

Taking the advantage of Eqs. (1) and (3) which were simplified to their forms for only one kind of particles in the CB, the electron band dispersion $E_{\mathrm{CB}}(q)$ may be determined. The calculations may be done in the analogous way to the analysis, performed previously for HH and LH minibands.

Because of narrow energy band gap of InAs the LH minibands affect the CB states. The effect is described with the help of the three-band Kane model which allows to treat the problem with the use of the modified effective masses of electrons and light holes [2]. The masses depend on the particles' energies and in the center of BZ are both expressed as $1/m = 1/m^{\Gamma}(1 + 2E/E_{\mathrm{G}})$, with $E_{\mathrm{G}} = 356$ meV denoting the energy band gap of InAs [3] (the plus in the expression for the LHs results from the model in Fig. 1a). The expression describing the modified effective masses is derived from the three-band Kane model in which the assumptions for the top of the valence band ($E_{\mathrm{V}} = 0$) and for the bottom of the conduction band ($E_{\mathrm{C}} = E_{\mathrm{G}}$) were made.

In order to solve Eq. (3) for LH and HH states the iterative procedure should be performed because m_{L} depends on E. Even though the HH mass is assumed the constant value m_{H}^{Γ}, still in the iterative procedure the miniband $E_{\mathrm{HH}}(q)$ is subtly modified by the reason of HH--LH interaction. The energy dependence of the effective electron mass (i.e. $m_{\mathrm{el}}(E)$) denotes that Eq. (3) written in the form valid for the electron states should be solved iteratively, too.

3. Results

Calculations were performed for the SL in which the thickness of the layers were $2a = 20$ Å and $2b = 40$ Å (Fig. 1). Simulations were done with the particle masses:

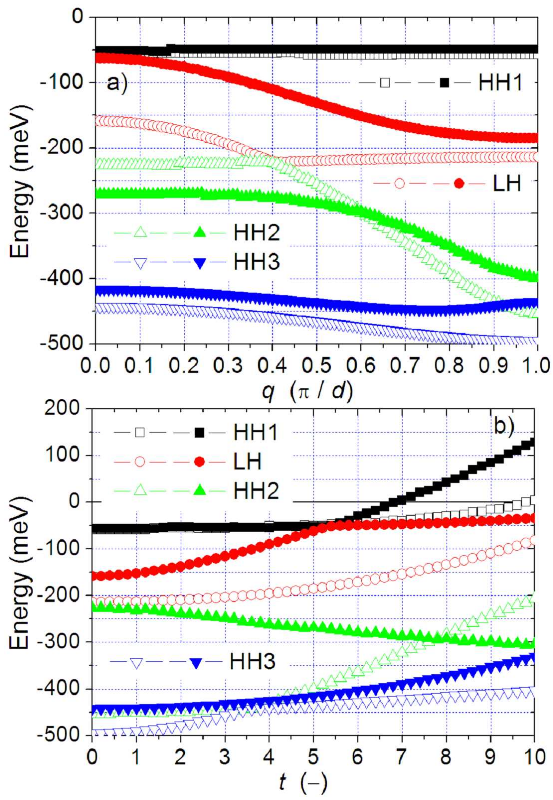

Fig. 2. (a) HH and LH band dispersions obtained for the SL with $2a = 20$ Å and $2b = 40$ Å. Dependences marked with the open symbols refer to $t = 0$. Filled symbols refer to $t = 5.0$. (b) Holes' energies versus the strength of HH–LH mixing at InAs/GaSb IFs. Filled symbols refer to the center of BZ. Open symbols refer to the zone edge ($q = \pi/d$).

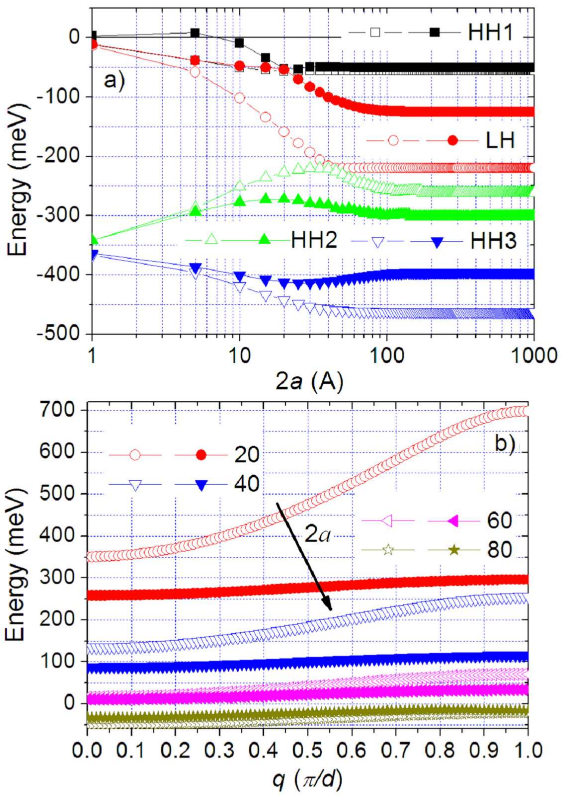

Fig. 3. (a) The energies of holes versus InAs layer thickness. The dependences are plotted in the center of BZ. Open symbols refer to the case of $t = 0$. Filled symbols refer to $t = 5.4$. (b) CB dispersions which include (filled symbols) and which do not include (open symbols) the nonparabolicity effect. $E(q)$ are presented for the SLs with $2a$: 20, 40, 60 and 80 Å. In all calculations GaSb layers had constant thickness $2b = 40$ Å.

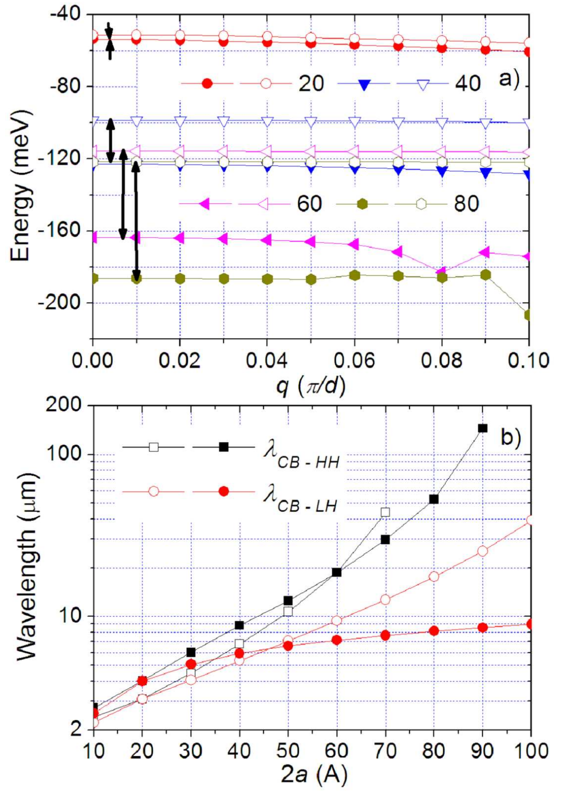

Fig. 4. (a) LH band dispersions for SLs with different InAs layer thickness, i.e. 20, 40, 60 and 80 Å. The dependences were calculated with (filled symbols) and without (open symbols) the respect of the nonparabolicity effect. The arrows mark the shifts of the electronic states caused by narrow InAs band gap. (b) Wavelengths corresponding to the interband transitions in the center of BZ. Curves were determined in calculations in which the nonparabolicity effect was (filled symbols) and was not (open symbols) taken into account. All simulations were done for the SLs with 40 Å thick GaSb layers.

$m_{\mathrm{L}} = 0.0247m_0$, $m_{\mathrm{H}} = 0.263m_0$ and $m_{\mathrm{el}} = 0.0183m_0$, where $m_0 = 9.11 \times 10^{-31}$ kg. HH and LH band dispersions calculated for two cases: $t = 5.0$ and $t = 0$ are presented in Fig. 2a. HH-LH mixing at InAs/GaSb IFs causes an essential change in the SL band structure. LH and HH2 minibands repeal and shift away from each other. It results in the LH miniband broadening and shifting it quite close to the miniband of HH1. Detailed analysis of HH1 band dispersion shows that in the case of $t = 5.0$ the value of $E_{\mathrm{HH}}(\pi/d)$ is slightly greater (by 2.34 meV) than $E_{\mathrm{HH}}(0)$, unlike in the case of $t = 0$. This may imply an indirect band gap of the structure (the similar result was pointed out in [1]). Such result seems to be nonphysical one particularly if the optical experiments regarding III–V materials are taken into account. The result obtained in the calculations inclines to verify the value of the experimental parameter t (in this work it was taken as in [1]).

In Fig. 2b $E(t)$ dependences are presented. Curves relating to $q = 0$ are compared to those for $q = \pi/d$. In the center of BZ the strongest HH-LH interaction is observed for $t = 5.4$.

Further investigations were performed to test the influence of InAs layer thickness on the SL properties. In these calculations GaSb layers had constant thickness ($2b = 40$ Å) and the value of $2a$ was changed up to 1000 Å. In Fig. 3a energies: $E_{\mathrm{HH}\,1}$, E_{LH}, $E_{\mathrm{HH}\,2}$, $E_{\mathrm{HH}\,3}$ in the center of BZ are plotted. Their dependences on the value of $2a$ are presented for $t = 0$ and for $t = 5.4$. Typical thickness of InAs layers in the SLs for infrared applications are from the interval $5 \div 15$ MLs (i.e. $30 \div 90$ Å). The values of $2a$ taken from this interval allow to control the top edge of HH and LH minibands.

In Fig. 3b the CB dispersions are presented. The width of the miniband and the values of allowed electron energies depend on InAs layer thickness. The minima of all plotted bands correspond to $q = 0$. Curves $E(q)$ are illustrated for two cases — if the effect of InAs narrow band gap is taken into account and when it is not considered. The narrow band gap of InAs causes the effect of nonparabolicity which means that the effective mass of the particle is not constant but depends on the particle's energy. The nonparabolicity effect causes an essential change in the CB dispersion — shifts the miniband down and makes it narrower.

The analogous effects are observed in Fig. 4a which refer to the LH's band. If InAs narrow band-gap effect is considered (Fig. 4a) the higher LH energies are obtained. Moreover, the thicker InAs layers denote the stronger nonparabolicity effects.

The calculated InAs/GaSb superlattice electronic structure gives the view on the possible interband transitions and corresponding wavelengths of the absorbed (or emitted) infrared radiation. In Fig. 4b the wavelengths versus InAs layer thickness are shown.

4. Summary

Electronic states of the type-II superlattice were calculated. The obtained results show that HH–LH interactions at InAs/GaSb IFs cause an essential change in the SL band dispersions. It was shown that the change of InAs layer thickness gives the possibility to control the band structure of the system. The thicker InAs layers cause the stronger nonparabolicity effect which results from the narrow InAs energy band gap.

Acknowledgments

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