THE ELECTRON STRUCTURE OF SAWTOOTH SUPERLATTICE

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Abstract

The band structure and interband matrix elements of $Al_xGa_{1-x}As$ sawtooth superlattice is analysed in this paper. We have shown that the envelope wavefunctions may be expressed as integral of certain elementary functions. Numerical results are given for superlattice with maximum mole fraction $x_{max} = 0.3$, and period equal to 14 nm. The agreement of our results with those obtained via pseudopotential method is better for higher values of conduction band offset ΔE_c. Transition matrix elements are strongly dependent on ΔE_c, which in principally enables determination of ΔE_c from optical absorption measurements.

1. INTRODUCTION

Multilayer graded-gap (sawtooth superlattice — STSL) have recently attracted great attention. In[1] F. Capasso et al. proposed a photodetector compraising this structure, taking use of the fact that electron and holes are spatially separated. Such a photodetector would have transient photoinduced voltage response of about 10 mV a decay time of 200 ps.

STSL has been treated in few papers. After the first paper[1], Jaros et al.[2,3] have analysed the minizone structure via pseudopotential method for zero transversal wavevector. J. A. Brum et al.[4] have calculated the electronic structure and time dependence of photovoltaic effect, however neglecting position dependence of

In this paper, we shall, within effective mass approximation, treat the band structure and envelope interband matrix elements, which is essential in analysis of this new class of high-speed, displacement current photodetector.

2. BAND STRUCTURE OF SAWTOOTH SUPERLATTICE

The $Al_xGa_{1-x}As$ STSL is a structure with linear variation of Al mole fraction $x(z) = x_{max}\ z/d$ within STSL period d. The graded Al concentration creates a potential which is a similar to an external electric field potential, with the difference that it concentrates the carriers on the same side of the heterointerface in both the valence and conduction bands (Fig. 1). The envelope wavefunction Schrodinger equation for electrons (and similarly for holes) within the effective mass approximation is:

$$-\frac{\hbar^2}{2}\frac{d}{dz}\left(\frac{1}{m^*(z)}\frac{d\psi}{dz}\right) + \left[U_e(z) + \frac{\hbar^2 k_t^2}{2m^*(z)}\right]\psi = E\psi, \quad (1)$$

where E is the total electron energy and k_t the transversal wavevector. For $x_{max} \leqslant 0.4$, the direct energy gap in $Al_xGa_{1-x}As$ varies linearly with x, thus U_e varies as az. As for the $m^*(x)$ dependence, there are two expressions currently used in the literature[5,6]:

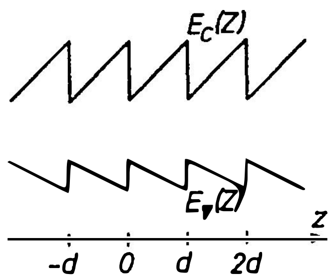

Fig. 1. Conduction-and valence-band profiles in STSL.

$$m^*_1(x) = m^*_{GaAs} + (m^*_{AlAs} - m^*_{GaAs}) \cdot x;$$
$$[m^*_2(x)]^{-1} = (1-x)\,[m^*_{GaAs}]^{-1} + x\,[m^*_{AlAs}]^{-1}. \quad (2)$$

If we assume the second expression in (2), after a lengthy calculation we get one particular solution of (1):

$$\psi_{p1}(y) = \int_0^{+\infty} \frac{ch[\sqrt{\epsilon_2}\ y\ th\ s - (\epsilon_1/\sqrt{\epsilon_2})\ s]\ ds}{ch\ s}, \quad \epsilon_1 \equiv \frac{2m_0}{h^2}\left(E + a\frac{B}{A}\right), \quad (3)$$
$$\epsilon_2 \equiv \left(+\frac{a}{A} + \frac{\hbar^2 k_t^2}{2m_0}\right)\frac{2m_0}{\hbar^2 A^2},$$

with the new varoable $y \equiv [m^*_2(x(z))]^{-1} \equiv B + Az$. The second linearly independent particulâr solution $\psi_{p2}(z)$, is to be determined by standard method[7].

If we use the first expression of (2), it is not possible to find particular solution in analytic form[8] and problem has to be solved numerically.

Applying the Bloch boundary conditions we get the dispersion relation $E(\vec{k})$:

$$\cos(k_z d) = \frac{1}{2}\left[y_1(d^-) + y'_2(d^-)\frac{m^*(d^+)}{m^*(d^-)}\right], \tag{4}$$

where $y_1(z)$ and $y_2(z)$ are the fundamental solutions of (1). The particular solution (3) and the fundamental ones are unuquely linearly dependent. Eq. (4) is valid even when discontinuity of $m^*(z)$ at the interface exists.

3. NUMERICAL RESULTS AND DISCUSSION

We calculated the band structure of STSL with same parameters as in[3] (d = 14 nm, x_{max} = 0.3). The spatial dependence of conduction (valence) band edges is given by[9] ($x \leqslant 0.4$):

$$U_{oe}\,[\mathrm{eV}] = 1.247 \cdot Q_e\, x_{max} \cdot \frac{z}{d} \text{ and } U_{oh}\,[\mathrm{eV}] = 1.247\,(1 - Q_e)\, x_{max}\,\frac{z}{d}, \tag{5}$$

where Q_e is the conduction band discontinuity energy gap difference ratio at GaAs $Al_xGa_{1-x}As$ interface. The data on Q_e vary considerably in the existing literature. We took values in range [0.60, 0.85] as reliable, although even values of 0.57 or 0.97 may be found.[10]

We get the best agreement between our results and those obtained via pseudopotential method for Q_e = 0.85 (for electrons). Our calculations of superlattice states at the center of Brillouin zone give energies: 125 meV, 222 meV and 307 meV, as compared to 140 meV, 270 meV and 310 meV pseudopotential values. For holes, however, the agreement is not that good; for Q_e = 0.85 we get energies: 19 meV and 35 meV (heavy holes) and 28 meV and 60 meV (light holes) while pseudopotential gives 8 meV and 30 meV, implying that the effective mass approximation is of low accuracy for holes. Furthermore, considering the pseudopotential results as accurate we conclude that Q_e = 0.85 gives the best results with effective mass approximation.

The envelope matrix element for interland transition is given by:

$$M_{env}(\vec{k}) = \int_0^d \psi_e\, \psi_h^*\, dz, \tag{6}$$

with envelope wavefunctions ψ_e and ψ_e normalized to unity within the STSL period. The dependence of $|M_{env}|^2$ (for k = 0) on Q_e is given on Fig. 2 for e-hh transitions.

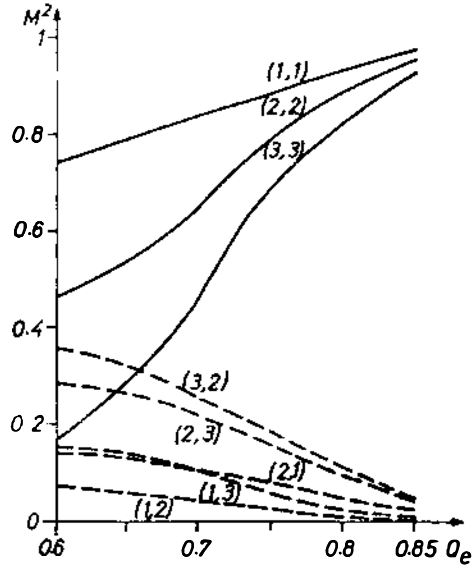

Fig. 2. The electron-heavy hole transition envelope matrix elements for STSL with d = 14 nm period and maximum mole fraction x_{max} = 0.3.

For higher values of Q_e (~ 0.85) transition matrix elements between minizones with same indices are nearly equal to unity, making that electron and hole wavefunctions have very similar forms. With decreasing Q_e these matrix elements also decrease, e.g. $|M_{env}|^2$ (Q_e = 0.6) = 0.18 for (3 — 3) transition. In case of transitions between different indices minizones, however, the opposite is true: $|M_{env}|^2$ increase with decreasing Q_e. The transition matrix element between third electron and first heavy hole minizones is considerably less then others ($|M_{env}|^2 \leqslant 0.04$ of all Q_e).

The electron — light hole transitions, the matrix element connecting same indices minizones increase with decreasing Q_e, and for $Q_e < 0.65$ they are very close to unity, while those for different indices minizones follow no simple rules (e.g. for (2 — 3) transition $|M_{env}|^2$ (Q_e) dependence has a maximum at $Q_e \cong 0.75$).

The dependence of $|M_{env}|^2$ on k_t and on choice of the wxpression for effective mass variation (2) is very slight, while the $|M_{env}|^2$ (k_z) dependence is roughly stronger if $|M_{env}|^2$ have lower values.

Finally, we propose that absorption measurement in STSL may be used for Q_e determination.

4. CONCLUSION

In this paper we analysed the electronic and optical properties of $Al_xGa_{1-x}As$ STSL. We derived analytical expression (3) for envelope wavefunctions in case of effective mass vs. mole fraction dependence given by the second expression in (2). Furthermore, we derived the dispersion relation (4) for SL having effective mass discontinuity at period boundaries, being the case in STSL.

We compare our results with those obtained via pseudopotential method, and found that the best agreement between the two is for $Q_e \sim 0.85$.

We have also calculated the electron-hole (light or heavy) minizones transition matrix element in STSL having period d = 14 nm and maximum mole fraction x_{max} = = 0.3. The numerical results indicate the essential matrix elements vs. Q_e dependence, implying the principal possibility of Q_e determination from light absorption measurements.

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