THE INFLUENCE OF CONTINUOUS SPECTRUM ON ELECTRON CONCENTRATION IN SEMICONDUCTOR QUANTUM WELLS

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Abstract

In this paper we analysed the influence of unbounded states on electron concentration in n-modulation doped quantum well. The expression derived for unbound electron concentration is general and applicable for any symetric structure with its potential vanishing at infinity. The influence of effective mass mismatch is also discussed.

The numerical results are given for GaAs quantum wells, 3 nm – 20 nm thick, at temperatures T = 77 K and 300 K. Relative concentration of unbound electrons is considerably for lower mole fractions x (independent of well thickness) and for longer values of x (for thinner wells). The results obtained may have implication on HEMT design.

1. INTRODUCTION

With the advent of the technology for creating high-quality quantum wells (QW) and superlattices has come a remarkably broad and promising vista of future new semiconductor physics and device applications[1]. Therefore, the nature of the electronic states in such structure is of great current interest, because semiconductor QW as known to efficiently collect carriers[2].

The first step of QW analysis is the determination of electronic structure. Papers concerning this subject mostly treated only the discrete part of energy spectrum, (bound states), which certainly is of greatest importance in some applications. The treatment given in[2] included unbounded states solved in a model system consisting of a single well surrounded by finite length barriers ending with infinite potential step (i.e. it deals with bound states of the full system).

In this paper we shall consider unbound states exactly, and also their influence on total electron concentration.

2. DETERMINATION OF ELECTRON CONCENTRATION IN QUANTUM WELL

A quantum well compraises a thin semiconductor layer (GaAs), tens or hundreds of angströms thick, imbeded in a higher band gap semiconductor bulk ($Al_xGa_{1-x}As$). Considering an n-doped structure, the hole concentration is negligible.

Initially, we consider the same structure as in[2], having only discrete states, and use the expression for local electron concentration[3]:

$$n(z) = \frac{1}{\pi} \sum_{i=0}^{+\infty} f_{FD}\, E_i\,(k_t^2)\ \psi^2_{i,k_t}(z)\, k_t\, dk_t, \tag{1}$$

where f_{FD} is the Fermi-Dirac distribution function, $E_i(k_t^2)$ — the i-th level k_t^2 dependence and $\psi_{i,kt}(z)$ the electron envelope wave function. With increasing L the number of states above the well increasis and that in the well remains constant for any definite k_t value (k_t is transversal wavevector). As $L \to +\infty$ the band spectrum, for energies above the effective potential barrier U_{eff} becomes continuous ($U_{eff} = U_o + [(\hbar^2 k_t^2)/2] \cdot (1/m_2 - 1/m_1)$, U_o — conduction band discontinuity, $m_{1,2}$ — effective masses in GaAs and $Al_xGa_{1-x}As$, respectivelly). We take that the well support s discrete levels at $k_t = 0$. As k_t increases, U_{eff} decreases because $m_2 < m_1$ and therefore the number of discrete levels decreases, untill for $k_t = k_{to} = 2U_o m_1 m_2/[\hbar^2\ (m_2 - m_1)]$ U_{eff} equals zero as well as the number of bound levels and only the continuous spectrum exists for $k_t > k_{to}$. Applying the box boundary conditions one can derive the expression[4] for total electron concentration (discrete and continuous spectrum parts):

$$n\,(z) = n_d(z) + n_c(z) = \frac{1}{\pi} \sum_{i=1}^{s} \int_{o}^{k_{ti}} f_{FD}(E_i(k_t^2)\ \psi_i^2\,(k^2{}_t, z)\, k_t\, dk_t + \\ + \frac{1}{\pi^2} \int_{o}^{+\infty} dk_z \int_{o}^{+\infty} f_{FD}\,(k_z, k_t^2)\, [\psi^2_{ec}\,(k_z, k_t, z) + \psi^2_{oc}\,(k_z, k_t, z)]\, k_t dk_t. \tag{2}$$

In (2) k_{ti} is the k_t value inducing the disappearance the i-th discrete level (certainly we have $k_{t1} = k_{to}$), and k_z is the wave vector component in QW direction. The continuous spectrum wavefunctions ψ_{ec} and ψ_{oc} having even and odd parity are normalized in such way tò take the form sin $(k_z z + n_{o,e})$ in the barrier material.

We also note that the $GaAs/Al_xGa_{1-x}As/GaAs$ („quantum barrier") structure has only continuous spectrum for $k_t = 0$ ($U_{eff} < 0$). However for large enough k_t the first bound level appears, and further increase of k_t even more levels appear. The expression (2) holds in this case upon substitution $s = +\infty$, $k_{ti} \to +\infty$ and lower limit in the first integral should be taken as k^*_{ti} (k^*_{ti} being the k_t value inducing the appearance of i-th bound level).

3. NUMERICAL RESULTS AND DISCUSSION

As numerical examples we give results for $Al_xGa_{1-x}As/GaAs/Al_xGa_{1-x}As$ QW having thickness 3 nm and 20 nm, at room and LN_2 temperatures. The electrons belonging to direct Γ as well as to indirect L and X minima were taken into account. The bulk parameters of host materials were taken from a recent review article[5]. The valence-band offset ΔE_v was calculated as $\Delta E_v[eV] = 0.55\ x$[6].

The average (taken over the well) relative unbounded electron concentration $\gamma_1 = \bar{n}_c/(\bar{n}_d + \bar{n}_c)$ vs. mole fraction x dependence is given in Fig. 1. For $x=0$ ($Al_xGa_{1-x}As$ bulk) γ_1 is certainly equal to unity as there are no bound states. With increasing x, γ_1 drastically decreases and for $x \cong 0.3$ majority of electrons populates discrete levels of Γ — minimum. For thicker wells (10 nm — 20 nm), γ_1 remains small (< 0.01) for all $x \geqslant 0.3$. For larger values of x, the direct electrons concentration in bulk become negligible as compared to that of indirect ones and Fermi level sinks deeply below conduction band edge E^{Γ}_c (in bulk). However, barrier hight U^{Γ}_o increases (the well deepens) and discrete levels decrease towards the Fermi level. The majority of bulk electrons populate X minima. The GaAs layer is the barrier for X electrons, so their concentration is very small here. For thinner wells (3 nm — 5 nm), however, we have a somewhat different situation because for larger x, Γ discrete levels are highly above E^{Γ}_c of GaAs (and Fermi level, too), implying a pronounced increase of γ_1 for $x \geqslant 0.6$ (T = 300 K) and $x \geqslant 0.8$ (T = 77 K).

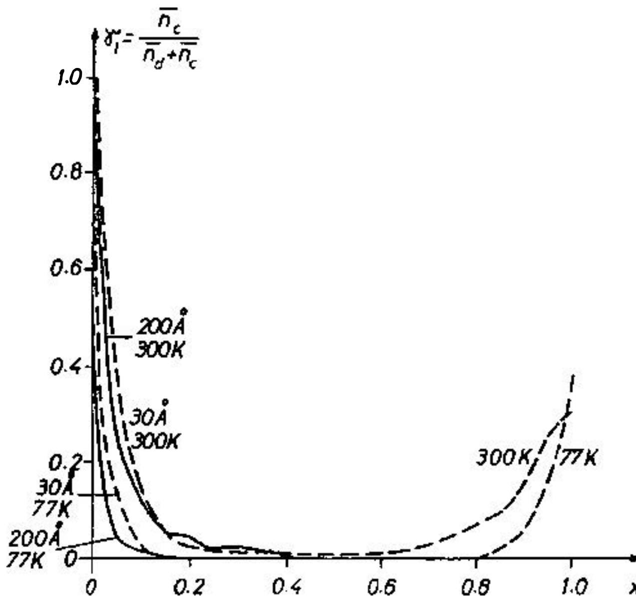

Fig. 1. The average relative unbound electron concentration vs. mole fraction x dependence for 3 nm and 20 nm thick QW in $Al_xGa_{1-x}As$ bulk n-doped to 10^{17} cm $^{-3}$.

4. CONCLUSION

A theoretical and numerical analyses of the influennce of continuous spectrum on electron concentration in n-doped QW is given in this paper. We derived the expression (2) for the total (bound and unbound) electron concentration, valid for any symmetric structure with vanishing potential at infinity. We discussed the influence of effective masses difference on electron concentration evaluation (appearance — or disappearance — of discrete levels one after another).

Numerical results are given for GaAs QW 3 nm and 20 nm thick imbeded in $Al_xGa_{1-x}As$ bulk and for T = 300 K and 77 K. The influence of unbound states is considerably for smaller values of mole fraction x ($x \leqslant 0.3$) but also larger x ($x \geqslant 0.6$ or $x \geqslant 0.8$) and thinner well, simultaneously.

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