STARK SHIFT AND FIELD INDUCED TUNNELING IN DOPED QUANTUM WELLS WITH ARBITRARY POTENTIAL PROFILES

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ABSTRACT

The energies and resonance widths of single doped quantum wells consisting of AlGaAs/GaAs with rectangular and annealing induced diffusion modified shapes are calculated under an uniform electric field using the stabilization method. The electronic structure is calculated without an electric field in the finite temperature density functional theory with exchange-correlation potential treated in the local density approximation. Our scheme for solving the Schrödinger and Poisson equations is based on the Fourier series method. The electric field is added to the self-consistent potential and energies are obtained as a function of the combined width of the well and barriers. This yields us the stabilization graph from which the energies and resonance widths at different field strengths are extracted using the Fermi Golden rule.

INTRODUCTION

There has been growing interest in using quantum wells (QWs) for optoelectronic device applications such as quantum well lasers, infrared detectors, wave guides and modulation doped field effect transistors[1,2]. The details of the electronic structures of the subband levels under the uniform electric field are necessary to understand the device performance. In an undoped sample the electronic structure of the subbands are described in the single particle picture where electron wave functions and the energy levels are completely decided by the barrier height and the well width. In a modulation doped QW the electrons flow from the barrier region into the well to bring the system to equilibrium. As a result of the higher density of electrons in the well, the Coulomb interaction between electrons becomes very important needing a complete many-body approach to this problem. In this case the subband energies and wave functions are dependent on the two-dimensional electron density and temperature.

Density functional theory (DFT) is a popular scheme for solving many-body problem. In this method the ground-state property of interacting electrons is determined by its charge density[3]. The many-body effects are taken in the exchange-correlation potential treated in the local density approximation (LDA). The single particle energies and wavefunctions are calculated using self-consistent Kohn-Sham equations[3]. This method has been applied to get energies and wave functions in the modulation doped rectangular QW[4]. However, the effect of the electric field on the electron subband energies and wave functions has not been addressed. A suitable method of extracting the mean tunneling times of the electrons under the applied electric field is not yet formulated. This paper attempts to use Fourier series technique[5] for the calculation of the energies, wave functions and mean tunneling lifetimes in the modulation doped rectangular and annealing induced diffusion modified QWs. For simplicity the conduction band shift due to the strain effect, nonparabolicity, depolarisation and exciton shifts[1] are not considered in this work.

THEORY

The self-consistent Kohn-Sham equation for calculating the energy E_n and wave function $\Psi_n(z)$ within the effective mass approximation in the Rydberg unit ($\hbar$=1, m_0=0.5

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and e^2=2) is given by

$$\left[-\frac{\hbar^2}{2}\frac{\partial}{\partial z}\frac{1}{m^*(z)}\frac{\partial}{\partial z}+V_{eff}(z)+eFz\right]\Psi_n(z)=E_n\Psi_n(z) \tag{1}$$

The effective potential (V_{eff}) is given by

$$V_{eff}(z)=V_{QW}(z)+V_H(z)+V_{XC}(z) \tag{2}$$

where V_{QW}, V_H and V_{XC} are the quantum confined potential, the Hartree potential and the exchange-correlation potential respectively. The Hartree potential is obtained from the Poisson equation

$$\frac{\partial}{\partial z}\epsilon_r(z)\frac{\partial}{\partial z}V_H(z)=4\pi e^2\rho(z) \tag{3}$$

where $\epsilon_r(z)$ is the relative dielectric constant along the z-direction and $\rho(z)=[n(z)-N_D^+(z)]$ with $n(z)$ and $N_D^+(z)$ as the carrier density and the ionised dopant density respectively. The carrier charge density at some finite temperature is given as

$$n(z)=2\sum_{n=1}^{n_b}\frac{k_BTm^*(z)}{\pi\hbar^2}ln\left[1+\exp\left(\frac{\mu-E_n}{k_BT}\right)\right]\mid\Psi_n(z)\mid^2 \tag{4}$$

where μ is the chemical potential. Integrating Eqn. (3) twice we obtain the Hartree potential as

$$V_H(z)=4\pi e^2\int_{-\infty}^{z}\frac{dz'}{\epsilon_r(z')}\int_{-\infty}^{z'}\rho(z'')dz'' \tag{5}$$

The boundary condition in this equation is that $V_H(\pm\infty)=0$. The zero temperature exchange-correlation potential (V_{XC}^0) in the LDA using parametrised form of Hedin and Lundqvist[6] is given by

$$V_{XC}^0(z)=-2\left[\frac{9}{4\pi^2}\right]^{\frac{1}{3}}\frac{1}{r_s}\left[1+\frac{0.7734}{21}r_s\left(1+\frac{21}{r_s}\right)\right]R_y \tag{6}$$

where $r_s=\left[3/4\pi a_0^3(z)n(z)\right]^{1/3}$, $a_0(z)=\epsilon_r(z)/m_r^*(z)$ and $R_y=m_r^*(z)/\epsilon_r^2(z)$ with $m_r^*=m^*/m_0$ The temperature is incorporated into the $V_{XC}^0(z)$ through[7]

$$V_{XC}(z)=\begin{cases}V_{XC}^0(z), & \gamma\le 0.15;\\ V_{XC}^0(z)\left[1+(a_1r_s^2+b_1r_s+c_1)\gamma^e/(a_1^*r_s^2+b_1^*+\gamma^d)\right], & 0.15<\gamma<12.\end{cases} \tag{7}$$

where $\gamma=k_BT/\mu$, a_1=-0.00388, b_1=0.04544, c_1=-0.443, a_1^*=1.5460, b_1^*=0.7023, e =2.04258 and d =1.80518. The chemical potential(μ) is obtained from the charge neutrality and depletion approximation conditions[4].

We have adopted the Fourier series method to solve the Kohn-Sham equation to obtain energies and envelope functions. Since the envelope function $\Psi_n(z)$ is a continuous function of z, it can be expanded into a truncated Fourier series of the form

$$\Psi_n(z)=\sqrt{\frac{1}{d}}\sum_k C_n(k)\exp\left(j\frac{2\pi k}{d}z\right) \tag{8}$$

where $j = \sqrt{-1}$ and d is the total length obtained by combining the width of the QW and barriers. Similarly $V_{eff}(z)$ and $1/m^*(z)$ and eFz are expanded in terms of the Fourier Series with coefficients $V_{eff}(k)$, $m(k)$ and $f(k)$ respectively. In terms of these coefficients the Eqn.(1) is derived as

$$\sum_i \left[-\frac{\hbar^2}{2} \left(\frac{2\pi}{d} \right)^2 m(k-i)ik + V_{eff}(k-i) + f(k-i) \right] C_n(i) = E_n C_n(k) \qquad (9)$$

The calculation of the chemical potential under the applied electric field is a complex problem to solve. It involves detailed knowledge of the field induced drift current and the tunneling current at the applied bias. For simplicity we have solved the DFT without electric field to obtain the quantum confined well shape and have then applied electric field on the well to study the Stark shift and resonance width.

The calculation of the energy shift and resonance width in a rectangular QW under uniform electric field by the stabilization method was developed by Borondo and Sánchez-Dehesa[8]. In the QW the energy levels calculated and plotted as a function of d show avoided crossings between stable and unstable eigenvalues at some points. The stable eigenvalues correspond to the energies representing the resonance position and the unstable eigenvalues correspond to the discretized continuum states. As an example, in Fig. 1 we present the stabilisation graph (SG) for a rectangular well at 100 kV/cm.

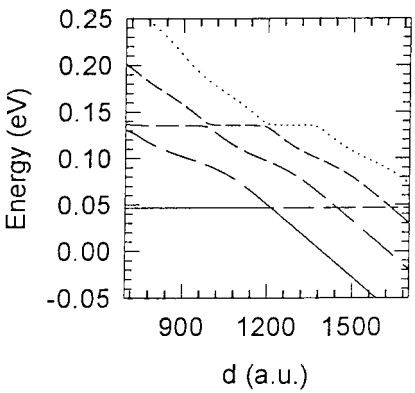

Fig.1
Stabilization graph of the rectangular quantum well with well width 100Å and $x = 0.3$ at the applied field strength 100 kV/cm. The energy levels for the ground, first, second, third, fourth and fifth excited states are denoted by solid, long-dashed, middle-dashed, short-dashed and dotted lines respectively. The avoided crossings are clearly seen here.

This graph presents avoided crossings between stable and unstable eigenvalues at different d_c for both ground state and first excited state energy levels. In the standard Fermi-golden-rule-type formula the resonance width (Γ)[8,9] is given by

$$\Gamma = 2\pi\rho(E_n)V_c^2 \qquad (10)$$

where the interaction term V_c is taken to be half the energy splitting at the pseudo-crossing (d_c) of the SG and $\rho(E_n)$ is the density of the continuum states. If E_n is the discretized continuum eigenvalue interacting with the stable one, a good approximation for $\rho(E_n)$ is[8,9].

$$\rho(E_n) = \frac{2}{E_{n+1} - E_{n-1}} \qquad (11)$$

To demonstrate its potentiality of the SG technique. We have applied it to two different types of well structures, namely the rectangular and the diffusion modified QW structures.

RESULTS AND DISCUSSIONS

I. Rectangular Single Quantum Well

The potential profile for a rectangular QW is given by

$$V(z) = \begin{cases} V_0, & \mid z \mid \geq L/2; \\ 0, & \mid z \mid < L/2. \end{cases} \tag{12}$$

where $V_0 = B_{off}(E_g(x) - E_g(0))$ with $E_g(x)$ and $E_g(0)$ the band gaps of $Al_xGa_{1-x}As$ and GaAs respectively. B_{off} is the band offset usually taken to be 0.7 and L is the width of the rectangular QW. The expressions for $E_g(x)$ and $m^*(x)$ have been given in our earlier work[5]. The width of the well is taken to be 100Å and $x = 0.3$ which corresponds to the barrier height of 295.6 meV. This well contains three bound states corresponding to energies of 32.07 meV, 126.51 meV and 267.88 meV. The barrier is doped with Si donors with binding energy 20 meV and concentration $2.5\times10^{20}cm^{-3}$. We have taken five eiteration to get full convergence in energy eigenvalues. The effective potential V_{eff} with and without the effect of the manybody terms is shown in Fig. 2. The chemical potential is found to be 107 meV. The concentration of the ionised donors corresponding to this chemical potential is found to be $9.3\times10^{16}cm^{-3}$. The energy levels are 54.59 meV and 133.44 meV.

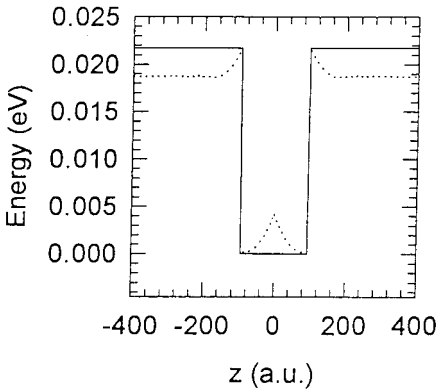

Fig.2
Potential profiles of the rectangular quantum well with and without modulation doping. The dotted line and solid line are the potential profiles with and without doping

The effect of the electric field on the energy levels with their resonance widths are given in Table 1.

Table I

Comparison of the energies and resonance widths with and without doping in a single rectangular QW. Energies with and without doping are denoted as $E_r^{(d)}$ and $E_r^{(w)}$ respectively. Similarly the resonance widths with and without doping are denoted as $\Gamma^{(d)}$ and $\Gamma^{(w)}$ respectively.

F (kV/cm)	$E_r^{(w)}$ (eV)	$\Gamma^{(w)}$ (eV)	$E_r^{(d)}$ (eV)	$\Gamma^{(d)}$ (eV)
50	0.03167	1.252×10^{-22}	0.05248	1.308×10^{-18}
100	0.02718	1.934×10^{-11}	0.04631	1.482×10^{-8}
150	0.02010	2.869×10^{-7}	0.03708	1.502×10^{-5}
200	0.01075	1.278×10^{-5}	0.02581	3.653×10^{-3}

From this table it is clear that energy levels and resonance widths are increased in the doped well compared to the undoped well. This happens because the barrier height is lowered as a result of the modulation doping in the rectangular QW.

II. Diffusion Modified Quantum Well

When the rectangular QW is subject to annealing above 800°C, intermixing starts at the heterojunction and the formation of the Ga vacancy induces Al atoms to diffuse into the GaAs layer from the AlGaAs [10]. The interdiffusion process is therefore characterized by the Al diffusion length ($L_d = \sqrt{Dt}$) which can be obtained from the diffusion constant (D) at the annealing temperature and the annealing time (t). Taking the diffusion constant to be isotropic, the position dependent Al concentration from the diffusion equation is found as[10,11]:

$$w(z) = x\left[1 - \frac{1}{2}\left\{erf\left(\frac{L+2z}{4L_d}\right) + erf\left(\frac{L-2z}{4L_d}\right)\right\}\right] \tag{13}$$

where erf is the error function[12] and L is the width of the rectangular QW. The potential profile is expressed as

$$V(z) = B_{off}[E_g(w(z)) - E_g(w(0))] \tag{14}$$

We have taken $x = 0.3$, L=100Å. The binding energy and concentration of Si dopants are the same in this case as in the rectangular QW. The diffusion length L_d=20Å. The chemical potential and the concentration of ionised donors calculated in the doped QW are found to be 52 meV and 4.17×10^{16} cm^{-3} respectively. The potential profiles with and without doping are shown in Fig. 3.

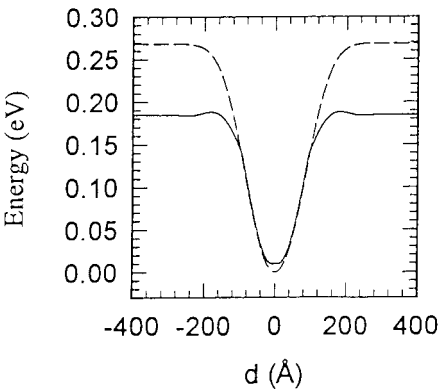

Fig. 3
Potential profiles of the diffusion modified quantum well with and without modulation doping. The solid line and dashed line are the potential profiles with and without doping.

The modulation doping has increased the effective width of the well and decreased the barrier height. The well before doping contains two energy levels at 55.63 meV and 160.46 meV. Since the barrier height is decreased in the doped well there is a single level in the well at 60.89 meV. The ground state energies and resonance widths for different field intensities are presented in Table II.

Table II

Comparison of the energies and resonance widths for a single diffusion modified quantum well with and without doping. The notations are the same as in Table I.

F (kV/cm)	$E_r^{(w)}$ (eV)	$\Gamma^{(w)}$ (eV)	$E_r^{(d)}$ (eV)	$\Gamma^{(d)}$ (eV)
25	0.028176	2.214×10^{-15}	0.060518	8.754×10^{-13}
50	0.027180	1.934×10^{-13}	0.059392	1.928×10^{-11}
75	0.020100	2.869×10^{-7}	0.057545	6.639×10^{-6}

As in the rectangular QW the energy levels and resonance widths are increased in the doped well compared to the undoped well. This happens because the barrier height is lowered as a result of the modulation doping.

CONCLUSION

In the present work we have extended the Fourier series method to calculate both the ground state quasi-bound energy levels with their resonance widths in the rectangular and diffusion modified modulation doped QWs. Although we have studied only two types of QW structures, this method can be applied to single, double and multiple QWs with arbitrary potential profiles. However, we would like to mention that this method cannot be used to study energies and lifetimes in QWs under a high electric field as the SG in this case cannot be obtained. We have not addressed the nature of quasi-Fermi level in the presence of the applied electric field in this work. The absorption coefficient in doped QWs under an applied electric field needs the temperature dependence of the Fermi level, wavefunctions, energies and mean tunneling lifetimes. Therefore our present work will be useful in calculating the absorption coefficients accurately in QW structures.

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