An Analytical model to determine the quantized energy levels and wave functions for Quantum Well devices

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We propose a physically based analytical compact model to calculate Eigen energies and Wave functions which incorporates penetration effect. The model is applicable for a quantum well structure (Fig. 1) that frequently appears in the state of the art nano-scale devices such as HEMT, MOS-HEMT, QW-FET, ETB, UTBB, DG-FET and so on[1-3]. This model is equally applicable for both silicon and III-V devices. The most attractive feature of our model is that, unlike other models already available in the literature, our model can accurately predict all the eigen energies without the inclusion of any fitting parameters. The validity of our model has been checked with numerical simulations and the results show significantly better agreement compared to the available methods.

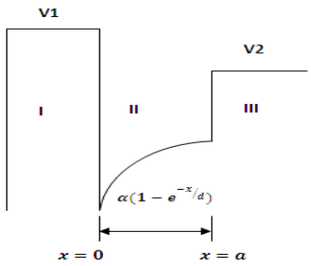

Fig.1: Quantum well under investigation

V1, $\alpha(1-e^{-x/d})$ and V2 are the assumed potential for the three regions in the structure of Fig. 1. Solving Schrodinger's equations, wave functions for the three regions can be represented as following:

$$\psi_1(x) = Ae^{\lambda x}u[-x] \quad (1)$$

$$\psi_2(x) = \left[B\,J_R\left(s\,e^{-x/2d}\right) + C\,J_{-R}\left(s\,e^{-x/2d}\right)\right](u[x]-u[x-a]) \quad (2)$$

$$\psi_3(x) = De^{\gamma x}u[x-a] \quad (3)$$

Where, $J_R(x)$ is the Bessel Function, $u[x]$ is the heaviside function and parameters λ, γ, R, s are defined as following:

$$\lambda = \sqrt{V_1 - E}/\mu \quad (4)$$

$$\gamma = \sqrt{V_2 - E}/\mu \quad (5)$$

$$R = \frac{2d}{\mu}\sqrt{\alpha - E} \quad (6)$$

$$s = \frac{2d}{\mu}\sqrt{\alpha} \quad (7)$$

Applying the appropriate Boundary conditions we get:

$$\lambda = \frac{\gamma P + N(R,a)N(-R,0) - N(-R,a)N(R,0)}{\gamma Q + N(R,a)\,J_{-R}(s) - N(-R,a)\,J_R(s)} \quad (8)$$

With,

$$P = \left[N(R,0)\,J_{-R}\left(s\,e^{-a/2d}\right) - N(-R,0)\,J_R\left(s\,e^{-a/2d}\right)\right] \quad (9)$$

$$Q = \left[J_R(s)\,J_{-R}\left(s\,e^{-a/2d}\right) - J_{-R}(s)\,J_R\left(s\,e^{-a/2d}\right)\right] \quad (10)$$

$$N(R,a) = \frac{d}{dx}\left[J_R\left(s\,e^{-x/2d}\right)\right]_{x\to a} = \frac{s}{4d}e^{-a/2d}\left[J_{R+1}\left(s\,e^{-x/2d}\right) - J_{R-1}\left(s\,e^{-x/2d}\right)\right] \quad (11)$$

Using the definitions we derive the following relations:

$$\lambda = \sqrt{\frac{V_1 - \alpha}{\mu^2} + \frac{R^2}{4d^2}} \quad (12)$$

Equating (8) and (12) and solving graphically we obtain the intermediate parameter R. The graphical solution of this equation yield multiple values for R, each value corresponds to one eigen state. The highest value of R yields the lowest eigen state. Eigen states are found with the following relation:

$$E = \alpha - \frac{\mu^2 R^2}{4d^2} \quad (13)$$

To validate the proposed model, a self-consistent simulator for DG-FET is designed which addresses the coupled Poisson's and Schrodinger equations[4]. DG-FET has the quantum well under consideration. Eigen energies are calculated using proposed model at various top gate bias and channel thickness. These results are compared with the self-consistent simulation results which show excellent agreement (Table I).

TABLE I. Eigen energies with $\alpha = 0.165\,eV$, $d = 5.328\,nm$

Eigen Energy	Self-Consistent Results (eV)	Proposed Model (eV)	% Error
1st	0.0671	0.0666	0.7%
2nd	0.1033	0.1047	1.3%
3rd	0.1269	0.1284	1.2%

The variation of different Eigen energies with the top gate bias is observed with a fixed channel thickness. Using the proposed model, the obtained wave functions $|\psi_1|^2$, $|\psi_2|^2$ and $|\psi_3|^2$ are plotted. The results are in excellent agreement with the self consistent results (Fig. 2 and 3).

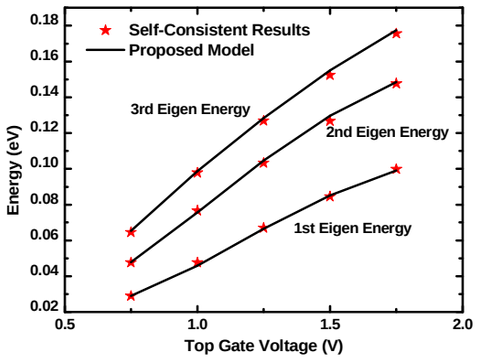

Fig. 2. Comparison of eigen energies

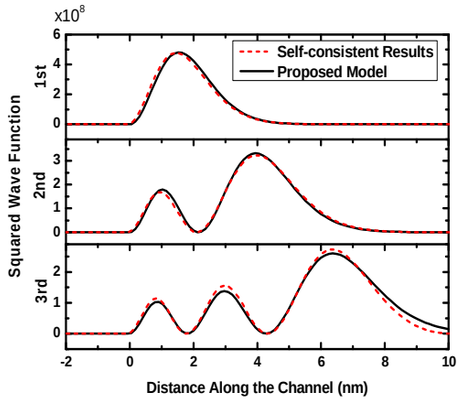

Fig. 3. Comparison of wave functions.

An accurate physics based compact model to calculate sub-band energies and wave functions has been presented here. The accuracy of the proposed model vastly depends on the extraction parameters α and d, whereas the value of these two parameters depends on channel doping and electric field.

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