A Theoretical Study and Modeling of Si/SiO_2 Multi Quantum Well MIS-Devices with Solving the Schrodinger-Poisson-Tunneling Current Equations Self-Consistently

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Abstract

In this paper, we investigate the model of a metal–insulator–semiconductor (MIS) device. Using this model, the current density–voltage (J–V) curves of MIS devices with single or multi silicon (Si) quantum wells (QWs) embedded between silicon dioxide (SiO_2) insulating barriers (Si: QW-MIS devices) are simulated. In the case of a single 4nm QW, we observe a step variation on current due to the rising of two first quasi-bound states in the QW above the conduction band edge of the Si substrate. By increasing the number of Si quantum wells to 3 and 5, this step increases since the first quasi-band states got broadened to mini bands. We demonstrate that by reducing width of the wells to 2nm the current step got disappeared. Effects of defects in the SiO_2 barriers are simulated indirectly by varying the electron effective tunneling mass in SiO_2. We observed a shift in the current step with reducing the effective mass of the SiO_2 barrier.

1. Introduction

Tunneling transport plays an important role in a wide field of applications involving charge carrier extraction through insulating Si-compound-based barriers or matrices. As model systems for the optimization of charge transport in Si quantum structures and as the central issue for efficient solar energy conversion and photo detectors, Si/SiO_2 multiple quantum well (MQW) structures with various thicknesses have been fabricated and studied [1].

The major difference between such Si/SiO2 and the well-known multi-layers based on III-V semiconductors is much larger potential barrier height limiting each well (around 3.2eV for electrons,4.4eV for holes). So, we need large electric fields to get a substantial current. Because of existence of this large barrier height, such Si devices behave more as a group of MIS capacitors put in series, work under large electric fields and connect to one another by tunnel barriers, rather than as what is generally expected from their III-V counterparts. As a result, these devices are planned to operate at high temperatures (300ºK and above) and it's also likely that such structures do not exhibit any quantum coherency from one well to its next nearest neighbors.

For electrical measurements on multi-barrier structures deposited on moderately doped Si substrates, it is important to determinate the Si substrate depletion layer width accurately, since a sizable voltage may appear across it relative to that across the multi-barrier structure. Since the device current is large enough to preclude thermal equilibrium in the Si substrate, a self-consistent solution is required that accounts for the dependency of carrier populations in the Si substrate on the magnitude of the device current. So we intend to introduce an accurate model to describe a MOS device that is not only capable of solving Schrodinger-Poisson-tunneling current equations self-consistently, but which allows the shape of the insulating barrier defined by the arbitrarily number of Si quantum wells. Such a model is useful in describing a range of MIS-based devices. For example, by modeling the insulator layer as a multi-barrier structure and applying a reverse bias, a MQW photodetector that is able to detect near UV photons have been introduced. Commonly, it's also reported that by considering the insulator layer as a double barrier structure, a system resembling an energy-selective contact to a bulk semiconductor could be achieved. This application is relevant to the field of contacts with energy-dependent transmission for the hot carrier solar cell concept [2]. We demonstrate that a multi-barrier structure has a larger step in its current curve in comparison with a double barrier structure and is more beneficial in this area of applications.

In the present study, application of Si/SiO_2 MQW structure in the forward bias situation has been studied. A self-consistent solution of Schrodinger, Poisson and current equations is employed. Current density-voltage (J-V) curves of MIS devices featuring an insulating layer comprised of 1, 3 and 5 Si QWs are presented.

2. Physical model of Si/SiO_2 MQW structure and its dominant equations

The structure under investigation is an Si/SiO*2* multi-layer composed of (1) a heavily doped polycrystalline Si with defined work function, (2) a series of undoped $SiO_2/Si/SiO_2$ quantum wells (we take 1,3,5 wells for comparison), (3) a bulk Si substrate with a given doping layer. The model is fully self-consistent, i.e. solving the Schrodinger-Poisson equation for the final charge distribution and energy states would give again the potentials and transmission coefficients which are efficiently used for determining the tunnelling currents.

The model is built around two basic assumptions that: (i) the hole tunnelling current through the insulating layer is much smaller than the current due to electron tunnelling, and (ii) the electron diffusion current at the edge of the depletion region is much larger than the generation-recombination current in the depletion region. Accordingly, the hole tunnelling current is ignored, and the net electron tunnelling current density ($J_{CM} - J_{MC}$) is equated to the electron diffusion current density at the edge of the depletion region (J_d) [3,5]. Fig. 1 depicts the band diagram of a MIS device featuring a multi-barrier structure as the insulating layer. The Si substrate is p-type and the top electrode is n^+ Si. Consequently the MIS device may be classified as the 'minority carrier' variety, with electrons being the minority carriers. A small negative voltage V is applied to the top n^+ Si electrode with respect to the p-type Si substrate. On account of assumption (i), the valence band edges of the multi-barrier structure have been intentionally omitted from Fig.1.

Assumption (ii), that the net minority carrier tunneling current is equal to the minority carrier diffusion current at the depletion region edge, can be expressed as:

$$J_{CM} - J_{MC} = J_d \tag{1}$$

We also write the below equations for diffusion current from [3]

$$J_d = q\sqrt{\frac{D_n}{\tau_n}}\left[n_s \exp\left(-q\psi_s/kT\right) - n_0\right]\coth\left(\frac{L}{L_n}\right) \tag{2}$$

$$n_s = N_C \exp\left(-q\Phi_{sn}/kT\right) \tag{3}$$

where the parameters n_s and n_0 are the conduction band electron concentrations adjacent to the Si surface (x=0), and at the back contact of the Si substrate, respectively. D_n is the electron diffusion coefficient, N_C is the effective density of states in the Si substrate conduction band, τ_n is the electron lifetime, L_n is the electron diffusion length and L is the total thickness of the Si substrate. The quantity Ψs is the electrostatic potential at the Si surface with respect to the back contact of the Si substrate, and $q\Phi_{sn}$ is the energy difference between the electron quasi Fermi level ($E_{F(n)}$) and the conduction band edge at the Si surface. The hole quasi Fermi level ($E_{F(p)}$) is approximated as uniform throughout the Si substrate, again because of assumption (i).

In order to make use of Eq.(1), an expression for the net electron tunneling current (J_{CM} - J_{MC}) is required. Ultimately such an expression may be obtained from [3,6]:

$$J_{CM} - J_{MC} = \int_0^{qXsc} J(E_x)dE_x = \frac{qm_0^*}{2\pi^2 h^3}\int_0^{qXsc} D(E_x,\psi_I)\times$$

$$\int_{Ex}^{qXsc}\left\{\frac{1}{1+\exp\left[\frac{(E+q\Delta-q\psi_s+qV)}{KT}\right]} - \frac{1}{1+\exp\left[\frac{(E+q\phi_{sn})}{KT}\right]}\right\}dEdE_x \tag{4}$$

In Eq. (4) m^*_0 is the transverse effective mass of electrons in Si, and $D(E_x, \Psi_I)$ is the probability an electron of longitudinal energy E_x will tunnel through the multi-barrier structure, across which an electrostatic potential drop Ψ_I occurs. E_x values rang from zero to the barrier height qX_{sc}. We take the point of zero energy ($E=0$) as the conduction band edge at the surface of the p-type Si substrate ($x=0$). To solve for the transmission probability $D(E_x, \Psi_I)$, we use an expression that links the applied voltage (V), with the potential drops across the multi barrier structure and the depletion region of the Si substrate (Ψ_I and Ψ_s respectively). Upon inspection of Fig. 1 a relationship between these quantities is readily obtained:

$$V = \Phi_m - \chi_{sc} - \Delta + \psi_s + \psi_I \tag{5}$$

The quantity Φ_m is the energy difference between the Fermi level in the top n^+ Si electrode ($E_{F(m)}$) and the barrier height, whereas qX_{sc} is the energy difference between the conduction band edge of the Si substrate and the barrier height. The energy difference between the Fermi level and the conduction band edge at the back contact of the Si substrate is given by q Δ.

The number of variables in the system comprised of Eqs. (1), (2), (3), (4) and (5) can be reduced by making use of the following relationship between Ψ_I, Ψ_s and Φ_{sn} [6]:

$$\psi_I = -\frac{d}{\varepsilon_{eff}}\operatorname{sign}(\psi_s)\sqrt{2kT\varepsilon_s}$$

$$\times\sqrt{N_A\left[\exp\left(-\frac{q\psi_s}{kT}\right) + \frac{q\psi_s}{kT} - 1\right] + n_s - N_C\exp\left[\frac{-q(\psi_s+\Phi_{sn})}{kT}\right]} \tag{6}$$

where ε_{eff} and d are the effective permittivity and width of the multi-barrier structure, respectively, ε_s the permittivity of the Si substrate and N_A the doping density of the Si substrate.

Typically in the case of a multi-barrier insulating layer, Eqs. (1),(2),(3),(4),(5) and (6) (from here on referred to as the system equation set) are combined to result in a single equation featuring only Ψ_s and Φ_{sn} as unknown variables. The equation is then solved numerically by first specifying Ψ_s through solving the Schrodinger-Poisson equations self-consistently, then iterating Φ_{sn} to find a valid solution. A consequence of iterating Φ_{sn} is repeated recalculation of $D(E_x, \Psi_s)$.This is necessary because changes in Φ_{sn} alter the electron concentration at the Si substrate surface, thereby changing the electric field in the insulating layer, and thus Ψ_I. Each time Ψ_I is varied, $D(E_x, \Psi_s)$ changes simultaneously. Consequently iteration of Φ_{sn} requires frequent recalculation of $D(E_x, \Psi_s)$ for each E_x value in a specified set.

Resonant electron tunneling coincides with population of QW quasi-bound states by electrons [7]. As discussed by Flynn et al. [5], establishment of the resonant tunneling condition involves a transient period where electrons congregate in the QW. Consequently this build-up of negative charge shifts the well upwards in energy, altering the electrostatic potential of the double barrier structure. Provided that the electron population in the cathode at the energy coincident to the new position of the

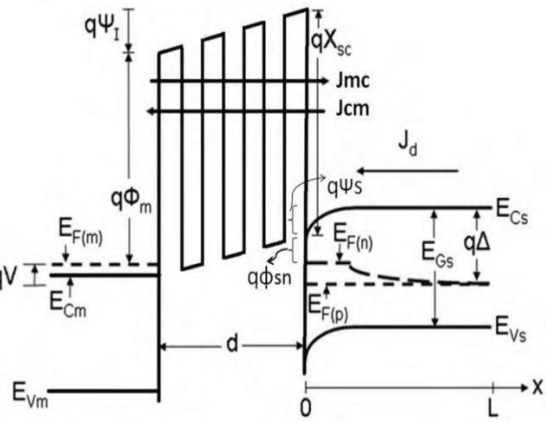


Fig. 1. Band structure of a MIS device featuring a multi-barrier insulating layer. The substrate is p-type Si and the top contact is degenerately doped n-type Si. The voltage (V) applied to the top n^+ Si contact with respect to the p-type Si substrate is negative. J_{CM}, J_{MC} and J_d represent conventional current densities.

quasi-bound state is sufficient to ensure it remains occupied, the resonance will be maintained. Indeed the upward electrostatic potential shift of the QW serves to make the multi barrier structure more transparent to tunneling carriers. Carrier trapping has been considered by our model in contrast with [5]. Consequently the transmission probability calculations are more accurate than would be obtained without a self-consistent solution of the Poisson and Schrodinger equations.

Fig. 2 demonstrates that the two approaches lead to calculation of different transmission probabilities for a single QW example. The positions of transmission resonances are virtually identical, with the difference in the position of the resonant transmission peaks and amplitudes. It should be negotiated that we cannot have any transmission probability for energies below 0.8 eV, since it's impossible for electrons with energies below the conduction band edge at the back contact of the p-type Si substrate (that is given by $q\Delta$), to have any resonance tunneling.

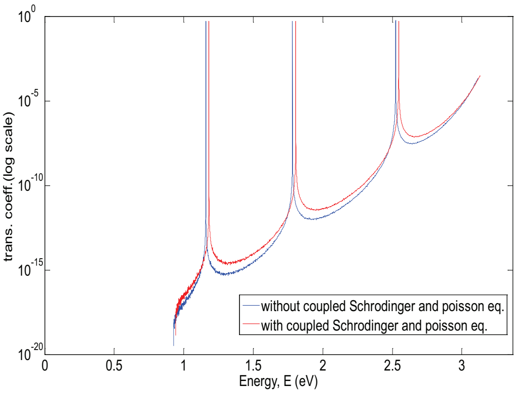


Fig. 2. Transmission probabilities of a single well structure, plotted as a function of carrier energy. The case of coupled Schrodinger equation is compared to the case of an uncoupled Schrodinger equation. The simulated SiO_2 barriers are 2nm in width, whereas the Si QW is 4nm. An applied bias voltage of 0.2 V exists across the structure.

3. J–V characteristics of a single and multi Si QW structure

Using the model described in the previous section, the J–V characteristics of MQW- MIS devices were simulated. For simplicity and also in order to compare our results with previous works [3, 5], we first modeled a QW double barrier structure consisted of 2 nm SiO_2 barriers either side of an intrinsic Si well whose thickness was varied between 2nm and 4nm. After that we changed our model to a 3 (Fig. 1.) and 5 quantum well structure to investigate the predictable changes in the tunneling current curves. The choice of effective electron tunneling mass in the SiO_2 barriers was based on the analysis of stadele et al. [8] accounting for complex bands and graded potentials at Si/SiO_2 interfaces via the effective electron tunneling mass. An effective electron tunneling mass of 0.43 m_0 was deemed appropriate for 2nm SiO_2 barriers. The value of electron effective mass in the Si QW was taken as $m^*_l = 0.92\ m_0$ and $m^*_t = 0.19\ m_0$, where m^*_l and m^*_t are longitudinal and transverse mass, respectively [8].

Fig. 3 shows the simulated J–V curves of Si: QW-MIS devices with 2nm SiO_2 barriers and QWs of varying thickness. Notably, a step occurs at about -0.45 V and another step occurs at about -1 V in the J–V characteristic of the Si: QW- MIS device with a 4nm QW. According to Flynn et al. [5], in order to understand the cause of the first step it is important to note that at zero applied bias there is a potential drop across the double barrier structure due to the work function difference between the n^+ Si top electrode and the p-type Si substrate. When a moderate negative bias is applied to the top n^+ Si electrode the potential drop is reduced, which shifts the quasi-bound states of the QW to higher energies (Fig 4). The step in the J–V curve of the 4nm Si: QW-MIS device occurs when the negative bias applied to the n^+ Si top electrode becomes sufficiently large to raise the first and second quasi-bound states of the QW above the conduction band edge of the p-type Si substrate. Consequently it becomes energetically favorable for electrons to tunnel from the n+ Si top electrode to the p-type Si substrate via the quasi-bound states. The high transmission probability associated with the quasi-bound states results in a steep rise in the device current. Fig. 4 illustrates the process graphically.

We observed another step which occurs at about -1 V in the J–V characteristic. In order to understand the cause of the second step it is important to note that when a high negative bias voltage (more than -1 V) is applied to the top n+ Si electrode the potential drop across the double barrier structure is increased, which changes our square potential barrier to a triangle potential barrier that cause the transmission probability increase, abruptly. In the other description, we can say that from this point our electronic transport mechanism changes from direct tunneling current to Fowler-Nordheim injection (tunneling from a triangle barrier).

It is also worthful to negotiate that the current step apparent in the J–V curve of the 4nm Si: QW-MIS device can be eliminated by reducing the width of the QW. It could be due to the increment of the energetic spacing between the Si QW conduction band edge and its first quasi-bound state. If the well width is made sufficiently small, the first quasi-bound states will be located above the conduction band edge of the p-type Si substrate at zero bias. So there is no state below the conduction band edge at zero bias and a current step will not occur due to the raising of the first and second quasi-bound state above it. In the case of a 3 nm QW the second quasi-bound state is positioned above the conduction band edge of the Si substrate but the first quasi-bound state is positioned below the conduction band edge yet, so we can again observe the step in current curve for lower applied voltages.

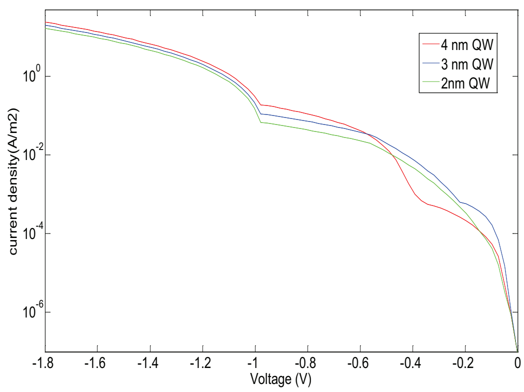
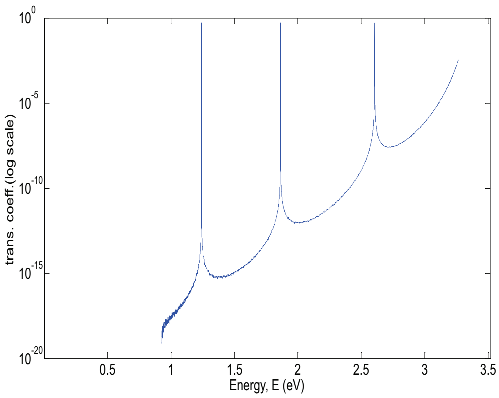
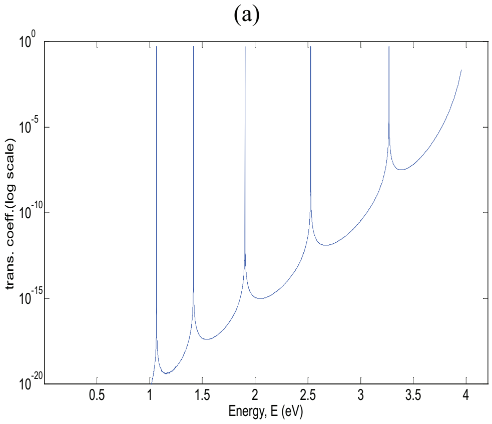


Fig. 3. Simulated J–V curves of Si: QW-MIS devices featuring 2nm SiO2 barriers. Curves are presented for QW widths of 2, 3 and 4 nm. The voltage was applied to the top n+ Si electrode with respect to the back contact of the p-type Si substrate.



(a)



(b)

Fig. 4. Si: QW-MIS devices under varying degrees of negative applied bias voltage. In diagram (a) the applied bias voltage is not large enough to lift the first (or second) quasi- bound state of the QW above the conduction band edge of the p-type Si substrate. For a sufficiently large negative bias voltage the first and second quasi-bound states rise above the substrate conduction band, as shown in diagram (b). Consequently the device current increases due to resonant tunneling of electrons via the quasi-bound states.

Until this point we simulate a double barrier structure, but now we try to apply our simulation model to a multi-barrier structure with a 3 and 5 Si QWs. Fig. 5 shows the simulated J–V curves of Si: 3 QW and 5 QW-MIS devices with 2nm SiO_2 barriers and 4 nm Si QWs.

After increasing the number of Si QWs to 3 and 5, the number of quasi-bound states increases, simultaneously and forms mini bands. In this situation when the first mini band of the structure comes above the Si substrate conduction band (with applying a sufficient bias voltage) a larger step in compare with a single well will observe since this time the width of the channels for electronic transport got thicker. Fig 6 illustrates the process graphically. As its observable in Fig. 4 and 6, in the case of a single well each state comprise of just one transmission peak, but in the case of 3 and 5 Si well each mini band comprise of 3 and 5 transmission peak, respectively. Having a larger step in current curve for multi-barrier structures is so worthful, because it resembles an energy-selective contact to a bulk semiconductor. This application is relevant to the field of contacts with energy-dependent transmission for the hot carrier solar cell concept [2]. The other important point about this curve is that the amplitude of current reduces with increasing the number of Si: QWs. It's predictable since the width of the whole SiO_2 barrier will increase by the number of Si: QWs, so it would be getting harder for electrons to have resonance tunneling through the barriers and the amplitude of transmission probability decrease although the number of resonance transmission peaks increase. It is also observable that the second step in current curve begins to disappear by adding the number of quantum wells.

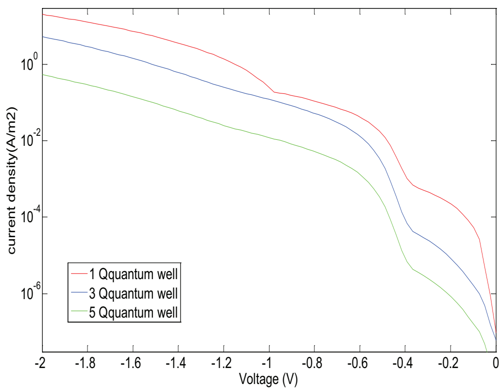
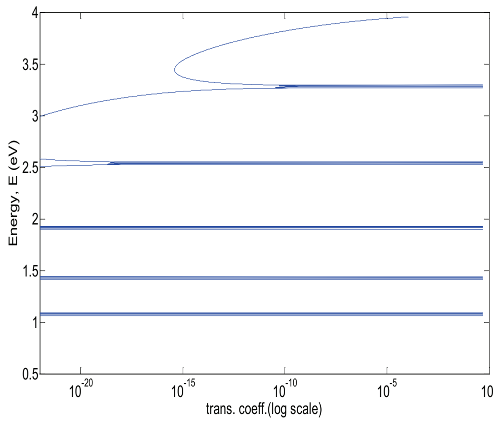
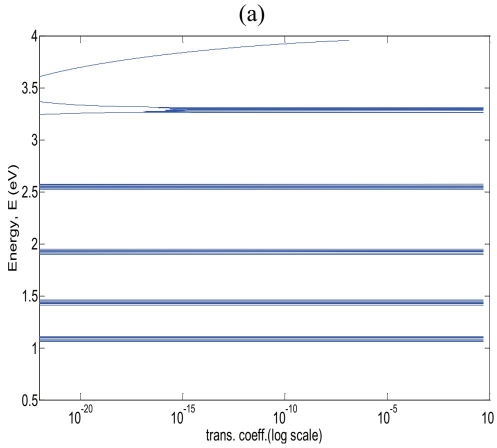


Fig. 5. Depicts the simulated J–V curves of Si: 1 QW, 3QW and 5QW -MIS devices with 2nm SiO2 barriers and 4 nm Si QWs.



(a)



(b)

Fig. 6. 3 Si QW (a) and 5 Si QW (b) - MIS devices under negative applied bias voltage of -0.9 V. The broadening of mini band is observable with increasing the number of wells.

The reason should be probably the large broadening of the forth and fifth mini bands of the multi well structure that decrease the possibility of observing an abrupt step in current and make it smoother.

By now, the electron effective tunneling mass in the SiO_2 barrier layers has been maintained at the constant value of $0.43m_o$. This value was deemed suitable for 2nm defect-free SiO_2 barriers [8], though in practice defects in the SiO_2 barriers may lead to smaller measured effective electron tunneling mass values. Obviously as the number of defects increases, the effective tunneling mass decreases due to defect-assisted tunneling. So we indirectly investigate the impact of SiO_2 defects by varying the effective tunneling mass to 0.32 m_0 and 0.22 m_0 for a structure with 3 Si QWS embedded in SiO_2 barriers. Fig 7 shows the J–V curves of this structure.

Reductions in the effective tunneling mass of electrons in the SiO_2 barriers alter the transmission probability of a 4nm multi Si: QW structure. So the amount of current increases, notably. It is consequent with a movement in the position of current step. In order to understand the reason of this movement in current step, we notice that a small effective electron tunneling mass causes the number of electrons that are injected from the top n^+ Si electrode to the Si substrate surface upon application of a negative bias voltage increase, these injected electrons prolong the presence of the inversion layer. Namely, the net build-up of positive charge at the Si substrate surface is diminished. Consequently the change in the potential drop across the multi-barrier structure is not as great. That is, a larger applied negative bias voltage is required to produce a given change in the potential drop across the multi-barrier structure. For more details we refer to Flynn et al. [5] that investigated a theoretical study for the reason of such shifts in J–V curves for double barrier structures.

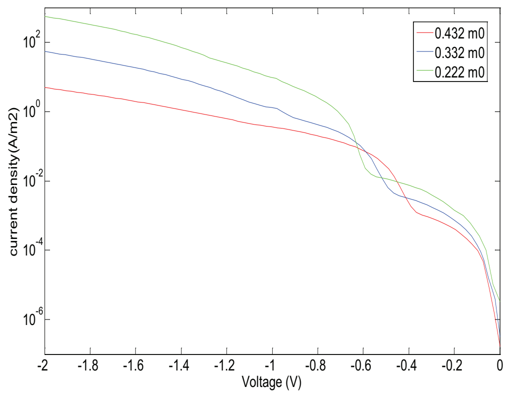


Fig. 7. Depicts the simulated J–V curves of a Si: 3 QW –MIS device with 2nm SiO_2 barriers and 4 nm Si QWs. Curves are presented for electron effective masses of $0.43m_0$, $0.32m_0$, $0.22m_0$.

4. Conclusion

We investigated a model for simulating Si/SiO_2 MQW MIS devices featuring multi Si QWs in the insulating layer. Such a model is capable to couple the Schrodinger-Poisson-tunneling current equations and solve them self-consistently.

Utilizing our model, J–V curves for Si/SiO_2 MQW MIS device with 4, 3 and 2nm QW widths were generated applying low bias voltages (less than 0.7 V in magnitude). We illustrated that for structures with 4nm Si QW width, there is a current step in the J–V curves caused by rising of the first quasi-bound state of the QW above the conduction band edge of the Si substrate. It has been demonstrated that the current step in the J-V curve moves to lower voltages for a 3 nm QW and disappear for a 2nm QW which could be due to the quasi-bound states shifts to higher energies and coming above the conduction band edge of the Si substrate in devices with narrower well widths. It has been shown that in a multi-barrier structure the current step increases with the number of Si quantum wells. Such event can be useful in a system resembling an energy-selective contact, i.g. hot carrier solar cell devices. Finally, we demonstrated the impact of SiO_2 defects on the J–V characteristic of a Si: QW-MIS device featuring 3 quantum wells in the insulator layer, indirectly by varying the effective electron tunneling mass in the SiO_2 barriers.

5. References

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