Current oscillations in semiconductor-insulator multiple quantum wells

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We examine theoretically the dc current-voltage characteristics of semiconductor-insulator multiple quantum wells with localized states in insulator barriers. The current exhibits periodic oscillating behavior for relatively high electric fields due to the resonant tunneling of electrons via these localized states. The time development of such current oscillations is also estimated. [S0163-1829(99)06847-2]

I. INTRODUCTION

Among attractive peculiarities of quantum wells there is the possibility to form a device with a negative differential resistance (NDR) based on resonant tunneling of the charge carriers.[1] The research interest in quantum wells historically focused on lattice-matched systems of $A^{III}B^{V}$ compound semiconductors.[2] Moreover, within the last decades $A^{III}B^{V}$-based multiple quantum wells (MQWs) have received special attention from both experimental[3–11] and theoretical[12–19] points of view, which focused on understanding the nature of the NDR. Extensive research has clarified the dominant mechanism of current transport in such systems to be sequential resonant tunneling.[6,20] In particular, the periodic current oscillations observed in MQW structures are due to the formation of a propagating high-field domain. The voltage drop across this domain aligns the first energy level of one well with the second energy level of the neighboring well, allowing resonant tunneling to occur. Additional voltage expands the high-field domain to include more and more quantum wells, with each added quantum well resulting in a current peak.

Presently there is a growing interest in the fabrication and the study of silicon-insulator MQW's related to their prospects in nanoelectronics and optoelectronics.[21,22] In Refs. 21 and 22, respectively, silicon dioxide (SiO_2) and calcium fluoride (CaF_2) were used as insulating materials. The electronic properties of these MQW's are quite different from those based on $A^{III}B^{V}$ structures. In particular, the barriers are much higher because of the larger band offsets in the silicon-insulator MQW's. Another relevant issue is the likely existence of localized states in the insulator barrier. The carrier transport behavior in such silicon-insulator MQW's is yet to receive extensive theoretical consideration, with only few studies reported to date.[23,24]

In this work we have attempted to extend the problem of the carrier transport in semiconductor-insulator MQW's to include a new effect. We suggest that in addition to direct tunneling through a barrier between two adjacent quantum wells electrons can also resonantly tunnel via localized electron states in the insulator. Thus additional periodic current oscillations may be observable in the current-voltage (I-V) characteristics of the structures. In the following, we first describe the model, which is then applied to Si/SiO_2MQW's and discussed.

II. FORMULATION OF THE PROBLEM AND THE MODEL

The structure we analyze here is a semiconductor-insulator MQW represented by the potential diagram in Fig. 1(a) for zero applied bias. It consists of N semiconductor quantum wells confined by $N+1$ insulator potential barriers. We suppose that our MQW structure is undoped and sandwiched between n-type electrode regions that are doped $N_D = 10^{18}\,\mathrm{cm}^{-3}$. Because of coupling between the quantum wells, a miniband is formed, but because of the high insulator barriers, this miniband is narrow. When an electric field is applied across the structure, the miniband breaks up in a ladder of localized ground states centered in the wells. In principle, due to energy and in-plane momentum conservation, charge transfer is possible only when the energy levels in adjacent wells coincide (resonant tunneling).[25] However, the existence of scattering mechanisms, such as interface roughness expected at a semiconductor-insulator interface, relaxes the in-plane momentum conservation rule.[26] The coupling to interface roughness is a rather complex problem, and its quantitative evaluation is beyond the goal of this paper. Therefore in the following we will evaluate direct tunneling between adjacent wells in the Wentzel-Kramers-Brillouin (WKB) approximation. For this we also assume that the characteristic relaxation time in the quantum wells due to phonon emission and interface scattering is faster than the charge transfer between wells due to tunneling (we will return to this point later in the paper). Thus it becomes possible to consider that the electrons relax down to the ground state of the semiconductor well before tunneling to the next one.

The new feature of our model is the presence of localized electron states within the barriers (Fig. 1). In silicon-insulator systems there can be different reasons for the appearance of such electron states in the insulator energy gap.[27] Namely, they can be related to (1) defects due to the stoichiometric distortion at the interface between silicon and insulator, (2) structural defects due to strained bond bridges

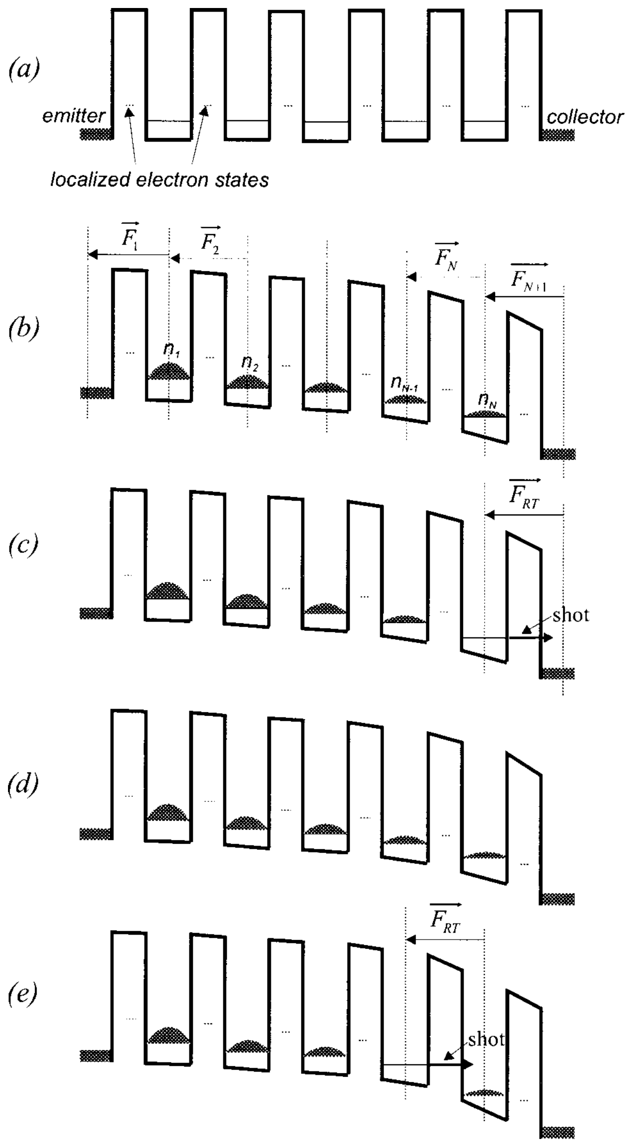

FIG. 1. Potential diagram of semiconductor-insulator MQW's with localized electron states within the barriers (a) in the absence (b)–(e) and under an applied external bias.

accommodating silicon and insulator layers, and (3) fixed charges in the insulator. We will treat these defects as traps with a Coulomb capture cross section. However, the qualitative features of the phenomenon are independent of the particular nature of these eigenstates. We assume, to simplify the model, that these states have the same energy position throughout the all barriers of the MQW's. However, the main predictions given by our model essentially hold if there is a distribution in energy of the localized states in the barrier. Since such states are usually found near the interface (~1 nm), the effective thickness of the insulating barrier covered by the model is not larger than 1.5–2 nm, which is in fact in agreement with the sizes dealt with in the experiments on silicon-insulator MQW's.[21,22]

As it has been shown in a number of papers,[15–19] charge transport in MQW structures can be described with rate equations for the carrier densities in the different quantum wells combined with the discrete Poisson equation; for example, see the work of Wacker *et al.*[18] The rate of change of the electron concentration in the ith well is described in the following manner:

$$\frac{dn_i}{dt}=g_{i-1}(n_{i-1},n_i,\vec{F}_i)-g_i(n_i,n_{i+1},\vec{F}_{i+1}). \tag{1}$$

Here the first term defines the tunneling flow bringing the electrons from the $(i-1)$th well to the ith one, while the second term is the tunneling flow withdrawing the electrons from the ith well to the $(i+1)$th one. Each term in Eq. (1) includes direct and reverse tunneling and as a function of carrier concentration n_i and electric field $\vec{F}_i$ is given by[28]

$$g_n^i=\frac{\sqrt{m_y m_z}k_B T}{2\pi^2\hbar^3 d_{\text{sem},i}}\int_0^U[F_{i-1}(E)-F_i(E)]dE\int_0^E T_i(E-E_\perp,m_x,\vec{F}_i)dE_\perp, \tag{2}$$

where $F_{i-1}(E)$ and $F_i(E)$ are the Fermi-Dirac distribution functions in the two wells; T_i is the tunneling probability; m_x,m_y,m_z are the electron effective masses in *x,y,z* directions; $d_{\text{sem},i}$ is the thickness of the ith semiconductor layer; $E_\perp$ and E are the transverse and total kinetic energy of electrons in the semiconductor; U_i is the barrier height for an electron in the ith layer; k_B is Boltzmann's constant; T is the absolute temperature (calculations assume $T=300\,\text{K}$); $\hbar$ is Planck's constant.

Charge carriers are provided and removed from the MQW system through contacts to the left and right. Within the model we assume that the applied bias and current through the system do not alter the properties of the emitter, which acts as a three-dimensional electron reservoir with a distribution density of $10^{18}\,\text{cm}^{-3}$. For the collector layer, given the appearance of a significant depletion region at large applied bias,[29] the electron density can be taken as zero near the barrier. Therefore, it becomes possible to model the contact layers by additional wells labeled 0 and $N+1$ with constant electron densities:

$$n_0=N_D,\quad n_{N+1}=0. \tag{3}$$

In order to describe a charge buildup at the ith well[30] we use the discrete Poisson equation connecting the fields at two adjacent wells $\vec{F}_i$ and $\vec{F}_{i+1}$ and the electric charge in the ith well:

$$\vec{F}_{i+l}-\vec{F}_i=\frac{ed_{\text{ins},i}n_i}{\varepsilon} \tag{4}$$

Here e is the electron charge; $d_{\text{ins},i}$ is the thickness of the ith insulating barrier; ϵ is the barrier permittivity. Note that in Eq. (4) we assume the voltage across one period of MQW's to drop mainly over the insulating barrier. This is reasonable, as the dielectric constant of an insulator is usually several times lower than that of a semiconductor (for instance, $\varepsilon_{SiO_2}=3.9$, $\varepsilon_{Si}=11.9$).

In the $2N$ equations (1) and (4) there are $2N+1$ unknown variables $n_i,\vec{F}_i$ $(i=1,2,...,N)$, and $\vec{F}_{N+1}$. One additional equation is the bias condition

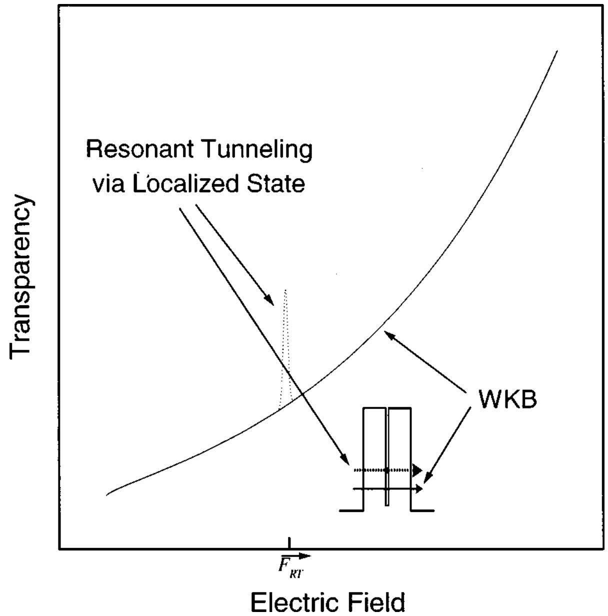

FIG. 2. Schematic transmission coefficient as a function of electric field for the barrier with a localized electron state.

$$\sum_{i=l}^{N+l} \vec{F}_i d_{\mathrm{ins},i} = V, \tag{5}$$

where V is the voltage applied to the structure.

Tunneling through a one-dimensional barrier containing available electron states has been analyzed already.[31,32] It was shown that the probability of tunneling is larger for the fields corresponding to resonant tunneling (RT) via localized electron states and was also proposed as one of the possible breakdown mechanisms of thin SiO_2 films. Therefore, these states can be modeled to exist in narrow wells inside the insulator barriers (see inset of Fig. 2). This implies that the function $T_i(\vec{F}_i)$ has a peak at an electric field $\vec{F}_{\mathrm{RT}}$ that aligns the localized state in the barrier with the electron energy in the well. We modeled such a peak by the Gaussian centered at $\vec{F}_{\mathrm{RT}}$:

$$G = \frac{A}{\sqrt{2\pi}\sigma} \exp\left[-\frac{1}{2\sigma^2} (\vec{F} - \vec{F}_{\mathrm{RT}})^2 \right] \tag{6}$$

and added it to the transmission coefficient defined by the WKB approximation (Fig. 2). The values $\vec{F}_{\mathrm{RT}}$ and σ serve as model parameters and depend, respectively, on the energy of the electron state in the barrier and the dispersion of its localization. If there are a number of localized electron states they should be modeled by additional peaks in the $T_i(\vec{F}_i)$ function. In Eq. (6) A is the scale factor representing the intensity of electron tunneling through the states in the barrier.

The I-V curve of the MQW structure is then calculated for a steady state by numerical integration of Eqs. (1) and (4) taking into account the bias condition (5). For simplicity we assume the barrier height for tunneling of electrons and the thickness of the insulating and semiconducting layers to be identical throughout the MQW structure.

III. RESULTS AND DISCUSSION

Two different types of the steady-state solutions have been studied. The first assumes that a uniform electric field exists across the MQW periods, i.e.,

$$\vec{F}_i = \vec{F} = \frac{V}{(N+l)d_{\mathrm{ins}}}. \tag{7}$$

Such a distribution makes physical sense only if the current through the MQW is negligible. The second case, which is closer to the real situation observed in experiments, corresponds to the nonuniform distribution, i.e., when different charge buildup in the wells results in different electric fields across the barriers. Solutions for both cases were considered for the MQW's consisting of 50 periods ($N=50$) of Si(1.4 nm)/SiO_2(1.5 nm). The conduction-band offset was chosen to be 3.0 eV.[33] The effective electron masses within silicon layer m_y, m_z were estimated from our previous band-structure calculations[34,35] to be $0.35m_0$. The electron effective mass in the tunneling direction m_x was assumed to be $0.42m_0$ as it was used in the calculations of Svensson and Lundström.[36] The energy of the ground state in the well was estimated using the numerical formalism proposed by Vassell, Lee, and Lockwood.[37] Simple estimations give that for the localized state positioned at 2.6 eV below the conduction band of the barrier,[38] the ground-state carrier energy in the well matches that of the eigenstate when the electric field across the insulating barrier reaches the value $\vec{F}_{\mathrm{RT}} = 8 \times 10^7$ V/m.

In the case of the uniform electric field distribution, the initial tunneling current is small and increases with the applied voltage. However, when the voltage reaches the value of $\vec{F}_{\mathrm{RT}} d_{\mathrm{ins}}\ (N+1)$ all the ground states in the QW's are in resonant conditions with the localized electron states in the insulating barriers. Thus, it gives rise to a sharp current increase. Once the voltage exceeds $\vec{F}_{\mathrm{RT}} d_{\mathrm{ins}}\ (N+1)$ the current decreases again, being limited by the WKB barrier tunneling transparency. The resulting static I-V characteristic is shown in Fig. 3(a). It has one current peak, whose amplitude and width are determined by the density of localized states in the barriers and their energy dispersion.

Now we proceed to the more realistic case when the electric field is distributed nonuniformly over the structure. Figures 1(b)–1(e) show the band scheme when a bias is applied to the device. When the applied voltage is increased from zero the electrons start to tunnel from one well to another, thereby producing a current that is defined by the WKB tunneling probability through an insulating barrier. The carrier tunneling leads to a space-charge buildup at the wells.[31] Thus, for a certain value of the bias voltage the electric field distribution over the structure becomes nonuniform as is shown in Fig. 1(b). The changing slope of the barriers is due to the different screening effect of the space-charge buildup.[31] The situation with the current changes radically when the voltage drops across the barrier closest to the collector $\Delta V = \vec{F}_{\mathrm{RT}} d_{\mathrm{ins},N}$ [Fig. 3(b)], i.e., when the ground state in the last well (Nth)E_1 is aligned with the eigenstate in the barrier E_s. Under these conditions a current shot is effectively created between the well and electrode, thus producing

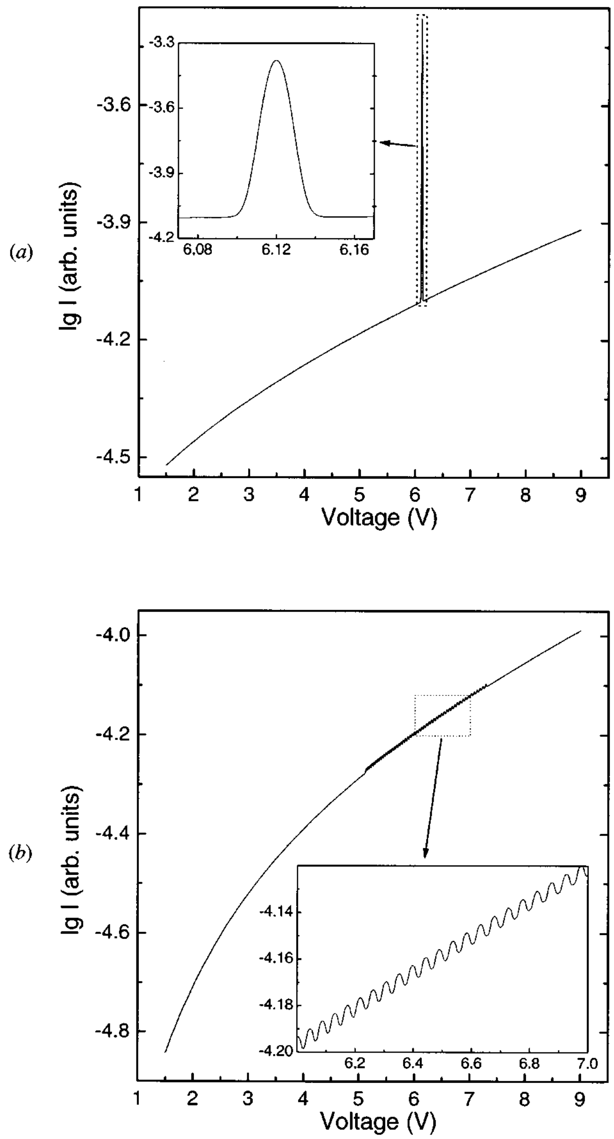

FIG. 3. Current-voltage characteristics of 50 periods of Si(1.4 nm)/SiO_2(1.5 nm) MQW's for (a) uniform and (b) nonuniform electric field distribution over the periods. In case (b) the field distribution is calculated self-consistently as described in the text.

the first current peak. Further increase in the bias will cause breaking of this resonant condition, thereby decreasing the current [Fig. 1(c)]. Then the eigenstate in the next barrier approaches the level of the ground state in the $(N-1)$th silicon well and the oscillation repeats [Fig. 1(d)]. The electrons from the ground state of the well tunnel via the localized state in the barrier to the adjacent well, followed by relaxation at the interface to the ground state of this well. As a result, one would expect $N+1$ current peaks for a device having N periods. The physical picture is quite similar to the domain formation in the $A^{\rm III}B^{\rm V}$ MQW structures studied previously.[18]

Figure 3(b) shows the static I-V curve calculated for nonuniform electric field distribution over the periods of the structure studied. There are indeed current oscillations appearing at an applied bias of 5.1 V and disappearing at 7.3 V. Another interesting point about the results presented in Fig. 3(b) is the period of the current oscillations. The formation of resonant conditions starts at the collector and propagates towards the emitter. However, due to the nonuniform electric field distribution over the structure, the voltage drop across the barrier (which is required to create the resonance) is not the same for the different barriers. Indeed it is smaller near the collector and greater near the emitter. Thus, the oscillation period increases with increasing bias.

As a final comment to the results, let us discuss the time development of the predicted current oscillations. This is an important point as far as the time-independent situation is considered within the model. However, it was pointed out elsewhere[29] for the high-conductivity state at the resonance to be fully established a certain amount of charge must be present on the resonant state. As in our case all localized eigenstates in the barrier are initially above the energy of the injected electrons; a transient time τ is required to accumulate this charge. This transient process can be estimated from simple consideration of RC delay of the ''quantum capacitor'' proposed by Luryi:[25]

$$\tau=\varepsilon\alpha^{-1}(\lambda/c)e^{4\pi d_{\rm ins}/\lambda}, \tag{8}$$

where $\lambda=h/\sqrt{2m_xU}$ is the de Broglie wavelength of the tunneling electron; α is the fine-structure constant; c is the speed of light. For the eigenstate located in the middle of the SiO_2 barrier 1.5 nm of thickness numerical estimations using Eq. (8) give τ to be of order of 10 ps. In contrast, the scattering times for Si/SiO_2 systems lie in the range of 0.1–10 fs depending on the mechanism and electron energy.[39,40] Therefore, the previously made assumption that electrons have time to relax to the ground state after tunneling into the next quantum well seems to be reasonable, as the scattering times are shorter than the effective charge-transfer time between adjacent wells.

IV. CONCLUSION

We have considered an added feature in charge-carrier transport across semiconductor-insulator MQW's: resonant tunneling between adjacent wells via localized electron states existing in the barriers. Single and multiple periodic current oscillations are predicted in the current-voltage characteristics of the structures for uniform and nonuniform potential distributions, respectively.

However, the experimental observation of such current oscillations can be difficult. Rather thin insulating barriers (<2 nm), as well as a high concentration of localized electron states, are required to provide the current at a resonance significantly higher than the current produced by interface-roughness-assisted tunneling of electrons through a set of insulating barriers.

The transport mechanism we analyze can be further developed to account for different localized states that are spread both in energy and space. Moreover, dynamic effects also seem to be interesting for further analysis.

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