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Transformation of a metal-insulator-silicon structure into a resonant-tunneling diode

G.G. Kareva ^{a,*}, M.I. Vexler ^b, Yu.Yu. Illarionov ^{b,c}

- ^a Saint-Petersburg State University, 3 Uljanovskaya, 198504 St.-Petersburg, Russia
- ^b Ioffe Physical-Technical Institute, 26 Polytechnicheskaya, 194021 St.-Petersburg, Russia
- ^cTU Vienna, Institute for Microelectronics, 27-29 Gusshausstrasse, 1040 Vienna, Austria

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ABSTRACT

A metal-oxide-semiconductor diode, with two tunnel-transparent barriers due to heavily doped silicon and nanometer-thin insulator, has been shown to exhibit steps or peaks in the static current-voltage curves. For the positive gate bias, appearance of these features in both simulations and measurements testifies to resonant tunneling of electrons from the silicon valence band via the discrete levels of the near-interface quantum well into the metal in the regime of deep depletion in silicon space charge region.

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1. Introduction

Metal-thin Insulator-Silicon (MIS) structures were being so intensively investigated within the last decades that their physics has already become a subject of some textbooks. Nevertheless a possibility of electron resonant tunneling (RT) between the metal and Si via the discrete levels in the near-interface quantum well (QW) has remained almost unknown so far. It is despite the fact that quantization effect itself was fully understood long ago [1]. In this work, the conditions for RT in MIS structures, modeling and experiments confirming its plausibility [2] are discussed.

Beyond an extension of knowledge in the physics of MIS structures, this study has an obvious importance in the applied physics and electronics. It should be noted that the two key branches of the modern electronics, namely, the Si integrated circuit electronics (despite scaling its elements toward nanometer size) and the low dimension functional nanoelectronics with its high speed components featuring non-linear characteristics, are developing rather independently. The materials, technologies and device design of the two branches almost do not overlap which gives rise to compatibility problem. Realization of a RT effect in a MIS diode would therefore become a step towards allying the above-mentioned branches and substantial extension of Si integrated circuit electronics functions.

In this work, for definiteness, the Al/SiO₂/p⁺-Si two-electrode structures are focused on. The samples were fabricated using standard technological processes and measured at 300 K. Calculations

were relied on the tunneling models [3] with the physical barrier parameters.

2. Conditions for a resonant tunneling in MIS nanostructures

In Fig. 1a, the calculated energy band diagram of the investigated nanostructure for the bias conditions enabling electron resonant tunneling from silicon, is presented for a case without any interface charges. There is a QW in the c-band (c = conduction) of the p^+ -Si with an energy depth value equal to the band bending ϕ_s which exceeds the silicon band-gap value E_g . The QW, being a part of the Si Space Charge Region (SCR), is sandwiched between the two barriers: of the remainder of the SCR from the one side and of the oxide from the other side.

The QW possesses many subbands, clearly distinguished in energy, which is essential for device operation, and level broadening which should be larger at higher temperatures is of no importance. Simulation of the band diagram was performed for the (100) orientation, for which there are overlapping ladders of heavy-electron (he) and light-electron (le) subbands [1]; the le-levels in Fig. 1 are drawn slightly wider to discern them from the he-levels.

The components of the flowing current are marked in Fig. 1b. Under the reverse bias considered the RT current $J_{\rm VM}^{\rm RT}$ is superimposed by the two non-resonant components. One of them arises due to a drift $J_{\rm d}$ of minority carriers (electrons) in the Si c-band through the SCR, balanced by their tunneling through SiO₂ into the metal ($J_{\rm cm}$). The other is created by electron tunneling from Si v-band through the oxide to the metal ($J_{\rm vm}$).

The RT electrons are emitted from a broad energy range of the occupied Si v-band states via the QW subbands into empty states of the metallic Al. The necessary condition for a RT is that at least

^{*} Corresponding author. Tel.: +7 (812) 4287153; fax: +7 (812) 4287240. *E-mail addresses*: galinakareva@mail.ru (G.G. Kareva), shulekin@mail.ioffe.ru (M.I. Vexler), illarionov@iue.tuwien.ac.at (Yu.Yu. Illarionov).

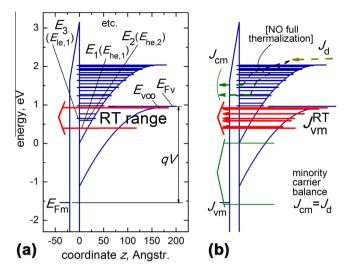


Fig. 1. Calculated band diagram of the Al/SiO₂/p⁺-Si RTD with oxide thickness d = 2.0 nm and acceptor concentrations $N_A = 10^{19}$ cm⁻³, under a positive gate bias V = 2.5 Volt (electron emission from silicon) with marked levels (a) and current components (b).

one of the QW levels must lie below the bulk v-band edge $E_{v\infty}$. According to the energy band diagram of the investigated structure, the RT from the Si starts with the lowest subband n=1, when the value of ϕ_s exceeds the value of E_g plus the energy E_1 of the first QW level. This means, that the RT process cannot come into effect at thermodynamic equilibrium in the SCR. A strong non-equilibrium in the depletion region is required, which is obtained in stationary regime due to a stationary current J_d . The condition for participation of the nth subband in RT is:

$$q\phi_{\rm s} \geqslant E_{\rm n} + E_{\rm g} \tag{1}$$

where E_n is the nth subband bottom energy. This subband gets activated at the voltage V_n^a warranting the exact equality in the expression (1), namely

$$V_n^a = q^{-1}(E_g + E_n) + U_n + V_{FB}$$
 (2)

with $V_{\rm FB}$ for the flat-band voltage and U_n for the insulator voltage at the moment of the subband activation. The values of U_n and therefore of V_n^a in case of SiO₂ are larger than they would be for high-K materials of the same physical thickness.

To observe RT at relatively low (several Volts) biases, the oxide and silicon forbidden-band barriers should be tunnel-transparent. For this purpose, aiming also at creating compact and high-speed MIS resonant tunneling diodes (MIS-RTDs, D = Diode), thin insulators (d within 0.4–4.0 nm) and high acceptor concentrations ($N_{\rm A} \sim 10^{19}~{\rm cm}^{-3}$) are used. The relation between the values of the transparencies of the two above mentioned barriers has a determining impact on behavior of the RT and its characteristics. In this paper, most results were obtained for the structures where the SCR barrier transparency $T_{\rm OX}$.

Evidently, the RT is possible only for a depletion or inversion operating mode and not for an accumulation when the band bending is always smaller than $E_{\rm g}$. So, for nanostructures based on n-Si under positive gate bias, no effect can be expected.

The second necessary condition for RT is that the averaged time τ_{sc} of inelastic scattering of an electron in QW must exceed the lifetime with respect to its tunneling through the oxide or the semiconductor forbidden band:

$$\tau_{sc} > \tau_{ar} (1 - (1 - T_{ox})(1 - T_s))^{-1}$$
 (3)

where τ_{ar} is a time between the sequential collisions of an electron with any barrier wall.

The condition (3) is a general RT transport requirement in any double-barrier-quantum-well system. If it is not satisfied, some electrons entering QW will lose their energies, which results in a partial break-off of RT. While τ_{sc} decreases, RT is replaced by another transport mechanism to be interpreted as a tunneling with destination in QW.

For a system with a small τ_{sc} compared to the right-hand side of (3), one can speak about electron thermalization in QW and introduce a quasi-Fermi level E_{Fc} for the well region of a MIS structure. At V>0, the c-band-metal non-RT component J_{cm} is then balanced not by the drift current J_d alone, but by the sum J_d+J_{bb} where J_{bb} is a band-to-band tunnel current in silicon, and no J_{VM}^{RT} exists. This situation looks more ordinarily for a MIS structure, although the existence of J_{bb} is also not often taken into account. The expression (3) may be treated as criterion for a transformation between the usual operation of a MIS structure and its operation as a MIS-RTD. Note that anyway the relation of $\tau_{sc} > \tau_{ar}$ must be presumed as otherwise there are no discrete quantum states.

Our further purpose will be to experimentally demonstrate a possibility of fulfillment of the requirement (3) and thus that a MIS tunnel structure can be forced to operate as a RTD. Evidently, this relies on an appropriate overall quality of the applied technology.

3. RT in Al/SiO $_2/p^+$ -Si diodes: modeling and experimental verification

Normally, for an Al/SiO₂/p⁺-Si system, the condition (1) can be satisfied only at positive gate bias V. As already said, the electrons are emitted from the occupied Si v-band states via the QW subbands into empty states of the metal (current J_{VM}^{RT}). Note that both electron-emitting and collecting regions are characterized by a broad energy range.

Fig. 2 shows partial contributions to a resonant current of each subband as calculated within the algorithm of Ref. [3], and Fig. 3 presents the full current–voltage (J-V) curves including all resonant and non-resonant components. Simulations are performed for two SiO_2 thicknesses.

RT activation in the MIS-RTD starts with the energetic alignment of the deepest (1st) subband bottom with the uppermost filled state in the v-band $E_1 \approx E_{V\infty}$. After the subband 1 has become active, it does not cease to operate with increasing bias V, thereby

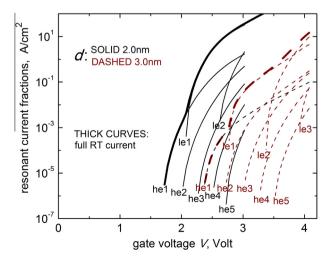


Fig. 2. Calculated partial RT currents, as functions of the gate bias, for several lowest QW subbands in the Al/SiO₂/p $^+$ -Si RTDs; acceptor concentration $N_A = 10^{19}$ cm $^{-3}$. The label "heN" ("leN") means transport via the N-th heavy- (light-) electron level

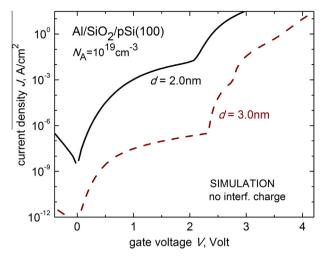


Fig. 3. Calculated current–voltage characteristics of the MIS-RTDs with the same parameters, as in Fig. 2. The total current includes both resonant and non-resonant (excess current) components.

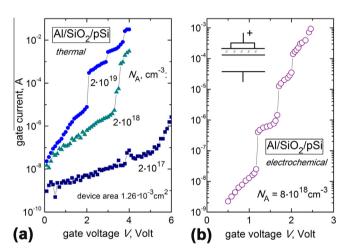


Fig. 4. Measured current–voltage characteristics (gate bias is positive) of MIS-RTDs: (a) with a thermal oxide and different Si doping levels; (b) with an electrochemical oxide.

the deeper filled states of the v-band are involved into RT. The result of this situation is steps (Fig. 3). Moreover, the shifts of the RT origin points enhance a band-to-band transport probability $T_{\rm s}(E_1)$ due to higher field and weaker SCR barrier within the tunneling distance. Meanwhile, the 2nd, 3rd etc. subbands are getting involved. Thus, at $V \geqslant V_n^a$, all n levels are taking part in RT simultaneously. Under these conditions, activation of the higher subbands is not always noticeable because they make their appearance on the background of the excess current $J_{\rm cm} + J_{\rm vm}$ and the current $J_{\rm VM}^{\rm RT}$ through already acting lower subbands (Fig. 3). Often, except the ground heavy-electron level $E_1 = E_{\rm he,1}$, the activation of only one more level, which is the first for the light electrons ($E_3 = E_{\rm le,1}$) is pronounced.

It is supposed interesting to estimate the maximal operating frequency of a MIS-RTD:

$$\omega_{crit} = (J_{vm}^{RT})^{-1} \sum_{n} \tau_{s,n}^{-1} J_{vm}^{RT,n}$$

$$\tag{4}$$

relying on the times of electron stay $\tau_{s,n}$ in the QW, which are given by the right side of the expression (3) calculated for each nth level. Estimations yield ω_{crit} in the teraherz range for the structures with d < 2.0 nm.

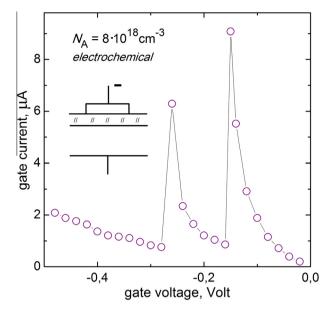


Fig. 5. Measured current-voltage characteristic of a MIS-RTD with an electrochemical oxide for negative gate bias.

For verifying a concept of RT in MIS tunnel structures, the samples with thermal and electrochemical silicon dioxide were fabricated and measured. The static current-voltage curves for the MIS nanostructures with a thermal oxide for several substrate doping levels are shown in Fig. 4a and a curve for the structure with an electrochemical oxide in Fig. 4b. In both cases the current-voltage characteristics exhibit step-like features. Although the form of the current jump segments is not exactly the same as in simulations, the features are difficult to attribute to anything else but to RT of electrons from the v-band of Si. For large N_A , such a behavior was typical for all examined diodes. A suspect that the jumps might be due to a peculiar oxide breakdown is removed by the fact of a complete repeatability of the features in several sequential I-V recordings for the same MIS sample (not shown). Note that the capacitance-voltage measurements on the "electrochemical" structures indicate a presence of some amount of a positive Si/ SiO₂ interface charge, which may lower the activation voltages V_n^a (i.e. shift them to the left).

These features, in their appearance, differ from the peaks observed in the J-V curves of the known RTDs [4]. This distinction between the RTDs and MIS-RTDs mainly results from a difference between the energy ranges of the electron emission in the compared devices. In the former case, when the peaks are observed, electrons are emitted only from a narrow energetic stripe, so that within a voltage range just after the resonance condition (i.e. an alignment of some QW level and this stripe) has been passed, current reduction takes place. In the latter case, the occupied Si v-band states over a broad energy range are getting involved in electron RT transport which occurs within the correspondingly broad voltage range.

Note that the resonance peaks can also appear if the electron-collecting energy range, instead of the electron-emitting one, is narrow enough. In principle, in MIS-RTDs, there is such a situation with an energetically narrow electron collector at negative gate biases (V < 0). Then it can be imagined that the electrons from the metal are tunneling via the QW levels into the empty v-band states. A reasonable amount of such states is available only slightly below the bulk valence band edge $E_{v\infty}$. Thereby, when $E_n \approx E_{v\infty}$ the RT peaks may appear. Electron tunneling into the much lower, filled states is improbable in accordance with Fermi statistics.

Theoretically, for the $Al/SiO_2/p^+$ -Si system with its regular band-offset parameters, it is not possible to fulfill the basic requirement

(1) for V < 0; consequently the above hypothetical RT-process seems to be excluded. However, some samples with electrochemical oxide demonstrate peaks (Fig. 5), which can be explained if some QW subbands may lie under $E_{v\infty}$ even at a negative gate bias. It should be noted that these features are making their appearance for relatively thick SiO_2 possessing positive Si/SiO_2 interface charges, and only after exposure of a MIS-RTD at V > 0 by the passage of some steps. Besides, the number of the discussed peaks under the polarity V < 0 is about the same as the number of the steps passed during a preliminary application of V > 0. In this case a form of the current–voltage curve depends on the program of voltage variation. These details may be related to the charging effects thanks to carrier localization in the QW in the course of electron RT from the silicon and their delocalization during electron RT from the metal. This phenomenon requires further study.

4. Conclusion

By presentation of the results of modeling and experimental investigations, the possibility for transformation of a metal–insulator-silicon capacitor into a resonant-tunneling diode has been shown. The energy band diagrams and the J–V characteristics of the Al/SiO₂/p⁺-Si(100) structures with Si doping level N_A of about 10^{19} cm⁻³ and SiO₂ thickness within 0.4–4.0 nm were discussed.

Novel MIS-RTDs are supposed to become a promising alternative to the traditional RTDs [4], based on the more complex materials and technologies not easily compatible with the MIS technologies. As compared to the previously reported Silicon-RTDs relying on the Al/SiO₂/Si/SiO₂/Si/Al [5] and CaF₂/CdF₂/CaF₂/Si [6] multilayer structures, or using the Si/SiGe systems (e.g. [7]), the proposed MIS-RTD is unambiguously simpler, that is one of its obvious advantages.

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