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PHYSICS OF SEMICONDUCTOR DEVICES

Adaptation of the Model of Tunneling in a Metal/CaF_2/Si(111) System for Use in Industrial Simulators of MIS Devices

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Abstract—An approach toward simplification of the model of the tunneling transport of electrons through a thin layer of crystalline calcium fluoride into a silicon (111) substrate with subsequent implementation in simulators of semiconductor devices is suggested. The validity of the approach is proven by comparing the results of modeling using simplified formulas with the results of precise calculations and experimental data. The approach can be applied to calculations of tunneling currents in structures with any crystalline insulators on Si (111).

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1. INTRODUCTION

Calcium fluoride (CaF_2) is a crystalline insulator; thin films of CaF_2 are successfully grown on silicon substrates with the (111) orientation thanks to the matching of their lattice constants. Previously, this fluoride was considered as an exotic material with questionable prospects of application in semiconductor devices. However, recently, progress was made in the technology of the growth of this material by the method of molecular-beam epitaxy and it was shown that it is possible to use CaF_2 for barrier layers in resonant-tunneling diodes (RTDs) and in superlattices (in combination with Si [1] or CdF_2 [2]). It is also worth mentioning that the old idea of using fluoride as a gate insulator in a field-effect transistor has become revived [3].

Results obtained in the sphere of technology naturally bring about a number of new problems in the area of modeling. Recently, we conducted calculations of the current–voltage (I–V) characteristics of metal–CaF_2–silicon structures without adjustable parameters [4]. The next stage consists in preparation for the use of commercial simulator programs for analysis of the behavior of devices with fluorite layers. The theory of tunneling transport through a crystalline insulator at the Si (111) orientation of a substrate is much more complicated than in the case of the (100) orientation, while simulators require considerable computational resources even in the case of Si (100). In order to reduce these requirements, it is necessary to optimize the model of tunneling; this is exactly the aim of this study.

In what follows, we suggest a simplified formula for the probability of tunneling and introduce an effective thickness of the CaF_2 film. In order to demonstrate the validity of the approach, we compare our results with exact solution and with the measurement data. In addition, we consider an example of one of the physical situations, for which the use of the simplified approach is intended (the case of a hot carrier leakage from the channel of a transistor with fluorite).

2. PARAMETERIZATION OF A MIS SYSTEM WITH CaF_2

The values of parameters for the CaF_2/Si barriers can be considered as reliably known. As in previous publications [4–6], we assume that the offset of the conduction band amounts to $\chi_e = 2.38$ eV and the offset of the valence band, $\chi_h = 8.6$ eV. The effective mass for both allowed bands of fluoride $m_e = m_h = 1.0m_0$ ($m_F = 1.2m_0$ for the Franz law). The low-frequency permittivity is equal to $\varepsilon_I = 8.43$, the band gap is $E_{gI} =$ 12.1 eV, and the electron affinity $\zeta_I = 1.67$ eV.

The height of the gold/CaF_2 barrier is $\chi_m = 2.63$ eV; this value was determined on the basis of an experiment with fabrication of metal–insulator–semiconductor (MIS) structures with fluorite. Taking into account the considerable excess of χ_h over χ_e and χ_m (see the left-hand side of Fig. 1), tunneling is always performed through the "upper" barrier and its probability is written as

$$T(E, k_\perp^2) = \exp\left[-2\hbar^{-1}\int\sqrt{2m_e(E_{cl}(z) - E + \hbar^2 k_\perp^2/2m_e)}dz\right] \quad (1)$$

including the cases of transport to (or from) the Si valence band. Here, E denotes the charge-carrier

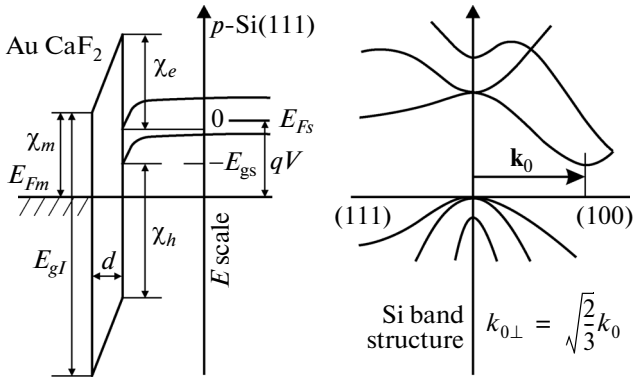

Fig. 1. Energy-band diagram of a MIS structure with CaF_2 (p-Si, accumulation mode). A fragment of the Si band structure is shown on the right.

energy, $k_\perp$ is the transverse (with respect to the transport direction z) component of its wave vector, and E_{cI} is the edge of the conduction band for CaF_2. The values of $k_\perp$ are large ($\sim k_{0\perp}$, Fig. 1) for electrons near the minimum of the Si(111) conduction band, while these values for holes near the top of the valence band are small; as a result, the hole current can compete with the electron current and must be taken into account.

3. STANDARD PROCEDURE FOR CALCULATING CURRENTS IN A MIS STRUCTURE

Approaches to the calculation of tunneling currents in a MIS system have been developed in fairly good detail [5, 6]. We now formulate the main aspects. In the most general form, the tunneling current is written as an integral taken over the total energy and the transverse wave vector:

$$j = \frac{q}{4\pi^3\hbar}\int(f_s(E) - f_m(E))dE\iint T(E, k_\perp^2)d^2\mathbf{k}_\perp; \quad (2)$$

here, f_m and f_s are occupancy functions for the available states in the metal and semiconductor (in the case of equilibrium carriers, the Fermi functions are used). However, the following formula has become the most conventional and most widely used in this context (see [5–7] et al.):

$$j = \frac{4\pi q}{h^3}\int \nu_\perp m_\perp(f_s(E) - f_m(E))dE\int T(E, E_\perp)dE_\perp; \quad (3)$$

here, integration is performed over the transverse energy $E_\perp$ (in addition to integration over E). The designations $m_\perp$ and $\nu_\perp$ denote the mass of the particle in Si in the plane of the structure and the degeneracy factor. The range of integration in (3) is determined by the presence of states with the given combination of E and $E_\perp$; it is worth noting that, in this representation, this range is divided into electron and hole regions. Transport from the surface levels can be taken into account introducing additional "discrete" terms [6], or by narrowing of the energy range in the quantum well, or using "quantum corrections" (a correction factor $\xi(E)$ in the integration over E, this is typical of simulators, see, for example, [8]). The complete algorithm for calculations was reported in [6].

The transition from (2) to (3) is admissible only for an amorphous insulator or in the case of the parabolic law of dispersion in a semiconductor and in the absence of a shift of the band extremum in the transverse plane ($k_{0\perp} = 0$). These are the cases of hole bands and electron bands for Si (100). However, in the case of a crystalline insulator on (111) silicon, we should average the probability over the states with the given pair of E and $E_\perp$ in order to use expression (3); in other words, we should substitute the following value (instead of T):

$$T^*(E, E_\perp) = \langle T(E, k_\perp^2(E, E_\perp, \alpha))\rangle_\alpha \quad (4)$$

(the parameter α represents the state in k space). Its obtainment is quite realizable individually [4] but is exceedingly cumbersome for a simulator, since it is required that additional integration be performed for each pair of E and $E_\perp$.

In calculation of the tunneling current through a layer of any insulator, it is necessary to take into account the final value of the root-mean-square deviation of the thickness σ_d:

$$\langle j\rangle = \int_0^{+\infty} j(d)\Gamma(d, d_n, \sigma_d)\delta d; \quad (5)$$

here, $\Gamma(d, d_n, \sigma_d)$ denotes the density of normal distribution with the nominal thickness d_n. This kind of distribution of thickness for CaF_2 was many times obtained by us using an atomic-force microscope. The above procedure is elementary but leads to a considerable increase in the calculation time.

4. OPTIMIZATION OF THE MODEL FOR IMPLEMENTATION IN A COMMERCIAL SIMULATOR

The main feature conditioned by the structure of the conduction band in silicon consists in the fact that the probability of tunneling decreases due to a large value of the transverse wave vector for electrons with energies E close to zero. As E increases, the effect becomes less pronounced and the situation becomes not much different from that in a direct-gap semiconductor. This is promoted also by the general complication of dispersion laws with increasing distance from

the minimum. In order to realize the idea using a mathematically simple method, we assume that the presence of component $k_\perp$, which is different for different states with given values of E and $E_\perp$, is equivalent to some shift ΔE of the energy of tunneling electrons. The largest shift ($\Delta E_0 = 2.44$ eV) is obtained at $E = E_\perp = 0$; we have $\Delta E \longrightarrow 0$ as the energy is increased. As a result, we write the expression for the tunneling probability for CaF_2/Si(111) in the following form:

$$T^*(E, E_\perp) = \exp[-2\hbar^{-1} \times \int\sqrt{2m_e(E_{cI}(z) - E + m_\perp m_e^{-1}E_\perp + m_0 m_e^{-1}\Delta E(E))}dz]; \quad (6)$$

here, the empirical relation

$$\Delta E = \Delta E_0 \exp(-E/E_s) \quad (7)$$

is suggested for the dependence $\Delta E(E)$. Expression (6) is then substituted into the inner integral in (3). The results of such calculations in comparison with those obtained using formula (2) (and using formula (3) with substituted (4)) yield the optimal value of 1.0 eV for the parameter E_s (Fig. 2a). The type of doping is not important in Fig. 2a since the argument there is the voltage across CaF_2. It is worth noting that, with $\Delta E = 0$, the relation (6) would acquire a "traditional" form, which is well known from many publications devoted to tunneling in MIS structures [6, 7].

We now consider the issue related to fluctuations in the thickness of the fluorite film. The presence of $\sigma_d \neq 0$ gives rise to a considerable increase in current as follows from calculations based on formulas (3)–(5) (Fig. 2b). Consequently, the effect under consideration cannot be disregarded. Instead, it makes sense to introduce an effective fluorite thickness as was done previously in the case of MIS structures with SiO_2 [9]:

$$d_{\text{eff}} = d_n - \eta\sigma_d^2; \quad (8)$$

here, η is the adjustable parameter, while d_{eff} is considered as the effective thickness of the homogeneous layer. This approach is based on the approximation $j(d) \propto \exp(-2\kappa d)$ ($\kappa = (2m_e\chi)^{1/2}\hbar^{-1}$) for the dependence of the local current density on the thickness; the density is "weighted" according to the Gaussian law (5). The quantity ~(3–3.5) eV can be taken as the characteristic barrier height χ. In this case, we take into account that typical voltages supplied to fluoride amount to about 1 V and that the barrier for holes is of the same order of magnitude as the barrier for electrons (we cannot disregard ΔE). In the case of realistic variations in χ, we obtain $\eta \approx 0.95$–1.00 assuming the quantities d_n, σ_d, and d_{eff} in (8) are expressed in angströms. As can be seen from Fig. 2b, the choice $\eta = 1$ ensures good fit, except for some difference in

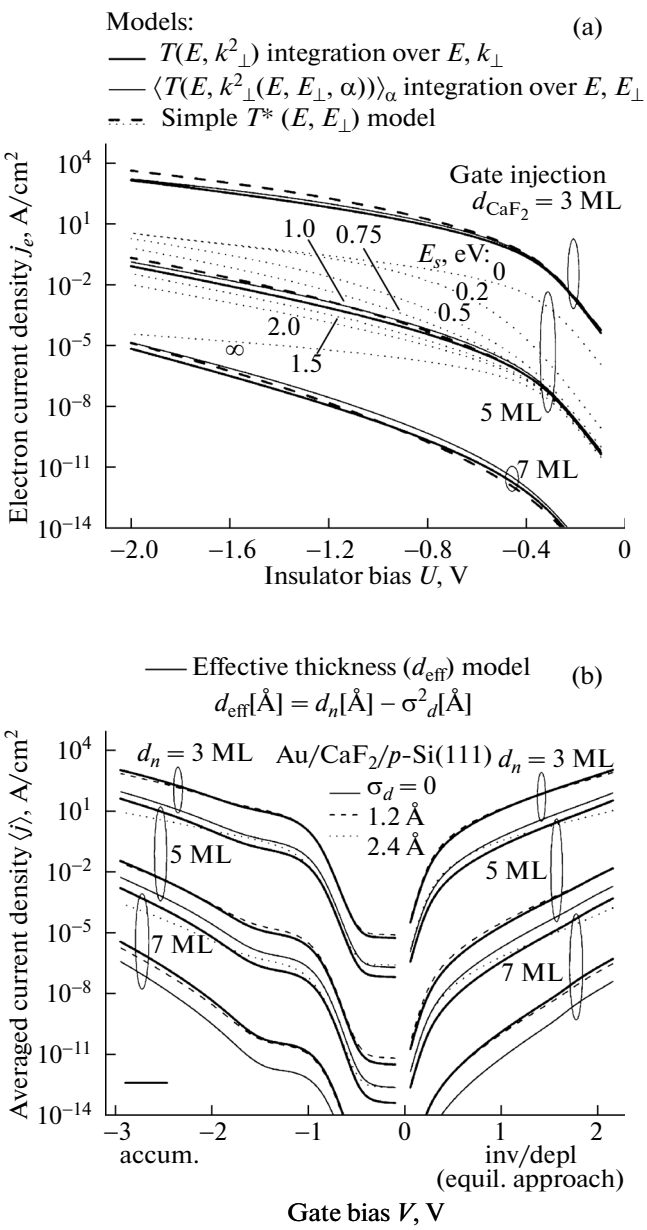

Fig. 2. (a) Selection of the parameter E_s, which characterizes a shift of the energy of electrons tunneling into Si (111); (b) calculation of current in the model of the effective fluoride thickness. 1 ML (monolayer) = 0.315 nm.

the slope of the curves. It is worth noting that the effect of fluctuations for CaF_2 is more pronounced (at the same σ_d) than for SiO_2 (in the latter case $\eta = 0.5$), which is related to a smaller effective mass ($0.42m_0$) [9].

It seems that the suggested simplifications (for T^* and d_{eff}) can be directly used in the implementation of semiconductor devices in industrial simulators. One such simulator can be represented in the near future by Minimos-NT [8]; its level meets the most stringent present requirements; however, this simulator has never been used for the devices based on calcium fluoride.

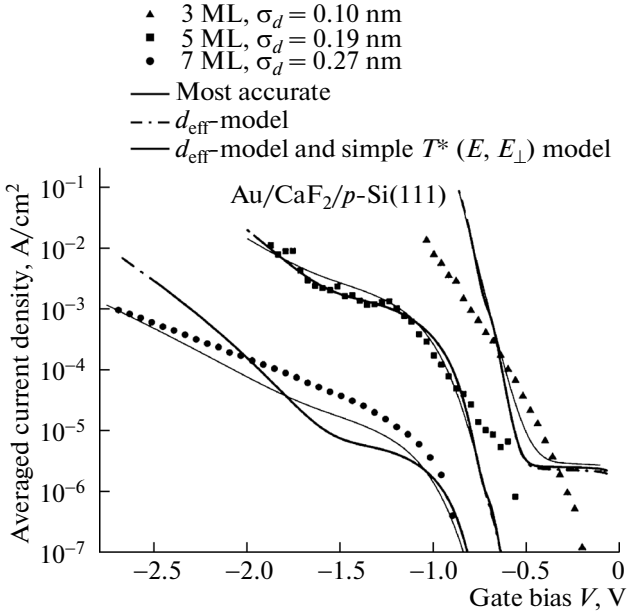

Fig. 3. Calculated characteristics of MIS structures with calcium fluoride in comparison with the results of measurements. The calculations were performed using three methods: exact (using formulas (3)–(5)), with the effective thickness (using formulas (3), (4), (8)), and using simplified formula (3) in combination with (6)–(8).

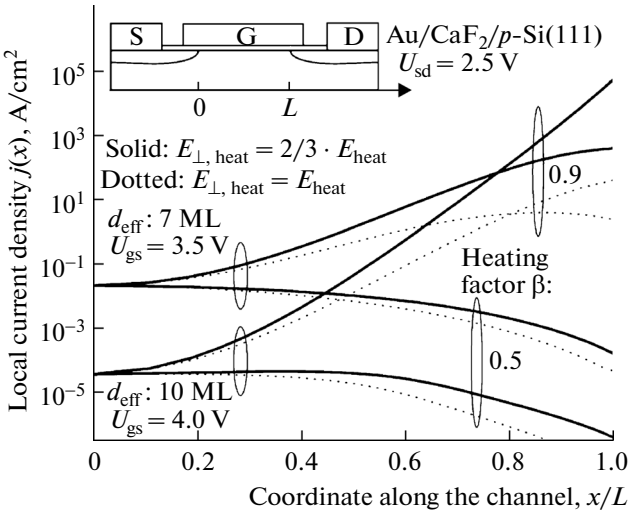

Fig. 4. Calculated tunneling leakages in the channel of a transistor with CaF_2 (taking into account the effect of "heating").

5. EXAMPLES OF CALCULATED CURRENT–VOLTAGE CHARACTERISTICS

Figure 3 shows examples of the current–voltage (I–V) characteristics for MIS structures Au/CaF_2/p-Si(111) ($N_A = 10^{16}$ cm^{-3}) in comparison with published experimental data [6]. The accumulation mode was chosen since interpretation of the data in the case of reverse polarity is complicated by the problem of a deficit of minority charge carriers [10]. Such results by themselves do not present substantially new information since an agreement was already obtained earlier (in the case of an accurate model). However, of main importance is the fact that the calculation was now performed also using an adaptive model suitable for simulators.

It is found that, in the latter case, calculations of the probability T^* and the effective thickness produce results which are in satisfactory agreement with those of precise calculations. It is noteworthy that deviations are mainly related to the use of d_{eff}, whereas the substitution of complicated averaging (4) with empirical formulas (5) and (6) barely gives rise to additional variations. Nevertheless, no doubt, relations (5) and (6) should be considered as those admissible for optimization of the model rather than those only possible.

It is worth noting that the range of thicknesses shown in Fig. 3 completely envelopes the region of practical interest: it is specifically ultrathin (with a thickness of two nanometers and less) fluoride layers that are required for RTDs, field-effect transistors, and injection MIS devices.

6. CALCULATION OF THE TUNNELING CURRENT OF HOT ELECTRONS

As an example of a real physical situation for the simulation of which an adapted model has to be applied with the use of an industrial simulator, we consider the case of hot electrons in the channel of a field-effect transistor. The cross section of such a device represents nothing else than a MIS tunnel structure.

Calculation of the leakage of hot charge carriers is performed using not the Fermi function for f_s in formulas (2) and (3) but the nonequilibrium distribution function, which is specific for each coordinate along the channel. This function is defined as

$$f_s(E) = dn(E)/dE\rho_{3D}^{-1}(E), \qquad (9)$$

where ρ_{3D} is the density of states in silicon and dn/dE (cm^{-3} eV^{-1}) is the energy distribution of electrons at the Si/CaF_2 interface. In order to determine dn/dE, we have to solve the Boltzmann transport equation, which requires considerable computational resources [11]. In connection with this, it makes sense to use optimized formulas in calculating tunneling currents.

Adequate simulation of the transport of hot electrons requires detailed analysis of the device's geometry, effects of scattering, and mobility. The simplest illustration in what follows serves only as a demonstration of the general plan. Let us consider an n-channel transistor (Fig. 4) with a CaF_2 layer. We designate the source–gate voltage as U_{gs} and the source–drain voltage as U_{sd}. We assume for the sake of simplicity that the difference in potentials between the gate and the

inverse layer varies quadratically with coordinate x on the straight source–drain line. The energy of heating behaves as $E_{heat}(x) = \beta q U_{sd} x^2/L^2$, where L is the length of the channel and β is a conditional factor, which varies in the range from 0 to 1. We also assume for simplicity that all electrons receive the same addition $E_{heat}(x)$ to energy at the source. In this artificial approximation, the function f_s at point x attains the "equilibrium" form with the shift of the Fermi level by $E_{heat}(x)$ for energies higher than $E_{min} + E_{heat}(x)$ and equals zero for smaller values of E. The quantity E_{min} is taken as the lowest electron energy at the source while the value of E at the point x relates to the bottom of the Si conduction band at this point.

We used formulas (3), (6), (7), and (9) in calculations of the current density (Fig. 4). It was assumed that the energy E_{heat} transforms by 2/3 (equal distribution over directions) or completely to $E_\perp$. Variations in the local current density $j(x)$ when approaching the drain are determined by the effect of heating, which induces an increase in $j(x)$ and by a decrease in the voltage applied to the insulator, which initiates the opposite effect. Naturally, at $E_{\perp heat} = E_{heat}$, the increase in the current with coordinate is less pronounced; however, even in this case, heating remains principally important due to the features of the CaF_2/Si(111) system since T^* increases all the same (see formula (7)). For insulators with thickness much larger than those in Fig. 4 and high voltages near the source, there is typically no leakage; however, the leakage increases steeply near the drain due to the overbarrier injection of electrons into the conduction band of the insulator (such situation, as occurring in a device with SiO_2, was considered in [12]).

7. CONCLUSIONS

In this study, we suggested a variant for the simplification of a model of the tunneling transport of electrons through a layer of crystalline calcium fluoride into Si (111) for use in industrial simulators of MIS devices. The validity of the model is proven by comparison with the results of precise calculation. The simplified approach can also be applied to MIS structures with other crystalline insulators on Si (111); the choice of CaF_2 is due to the fact that, for this insulator, experimental confirmation of importance of studied tunnel-transport features has already been obtained. An extension of this study should consist in carrying out calculations using simulators for specific devices with fluoride films at the same mathematical level at which calculations are performed for more conventional insulators.

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