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Fluctuations of the surface potential in metal–insulator–conductor structures

V. A. Gergel' and R. A. Suris

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The potential relief of the semiconductor–insulator interface, due to the inhomogeneity of the charge in the insulator, is investigated in MIS structures. Assuming no correlation between the positions of the charged centers and taking into account charge-density fluctuations of all scales, the mean squared fluctuations of the surface potential are determined as functions of the character of the location of the built-in charge in the interior of the insulator and of the electron density. The effective density of the surface electronic states due to the potential fluctuations is obtained, as well as the temperature dependence of the surface conductivity of the MIS structure.

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In the overwhelming majority of cases, the threshold voltages of the characteristics of MIS (metal-insulator-semiconductor) structures and of devices on their basis are shifted as a result of the presence of a certain fixed charge in the insulator layer. This "built-in" charge causes a corresponding bending of the bands in the surface region of the semiconductor in the absence of an external bias. Its magnitude is characterized by the so-called flat-band voltage, i.e., the voltage that must be applied to the metallic electrode of the structure to compensate for the action of the built-in charge on the semiconductor. It is clear beforehand that the density of the built-in charge is not uniform over the area of the MIS structure. One of the causes of the inhomogeneity is the imperfection of the methods used to prepare the MIS structure. However, even at the most perfect technology, there remain statistical fluctuations due to the discrete character of the elementary charge. The inhomogeneity of the built-in charge, causing corresponding fluctuations of the surface potential of the semiconductor, can lead generally speaking to much more substantial changes of the capacitive and current characteristics of the MIS structures than a simple additive shift along the voltage axis. In fact, consider by way of example an MIS structure at $T = 0$, in which the average surface potential corresponds to depletion of the majority carriers from the surface layer (see Fig. 1). The Fermi level on the surface lies in this case much lower than the average position of the bottom of the conduction band. In the homogeneous case the surface concentration of the carriers at such a bending of the bands would be zero. However, because of the inhomogeneity of the built-in charge, the position of the edge of the band fluctuates, and the bands cross the Fermi level in individual sections of the surface. In these sections, a certain electronic charge is accumulated, so that the average electron density becomes finite. It is clear that with increasing bending of the bands the fluctuation amplitude needed for the formation of the electron "drop" decreases, the probability of such a crossing increases, and the average electron density increases. The actual situation is somewhat more complicated, since the amplitude of the fluctuations is, on account of screening, itself dependent on the electron density, whose value must be determined in self-consistent fashion. The electrons, which accumulate in the minima of the potential relief, partially screen the semiconductor volume, and this decreases the total-voltage fraction across the space-charge layer, and leads therefore to an increase of the capacitance of the MIS structure, similar to what occurs when the surface states are filled.[1] Thus, one of the experimental manifestations of the fluctuations of the built-in charge may be deformation of the $C-V$ characteristics of the MIS structure.

Another manifestation of the fluctuations of the built-in charge is a characteristic dependence of the surface conductivity on the temperature and on the bias voltage. In fact, when fluctuations are present the surface electrons are located mainly at minima of the surface relief. Therefore the flow of current in the system requires the surmounting of potential barriers, and

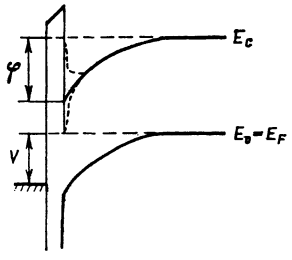

FIG. 1.

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this leads to an activation dependence of the conductivity on the temperature.

The foregoing qualitative arguments concerning the role of charge fluctuations are similar to those used in Refs. 2 and 3, devoted to fluctuations in the interior of strongly doped semiconductors. Our problem however, has a number of important distinguishing features. First, in contrast to the three-dimensional case, the mean squared fluctuation of the potential does not become infinite even in the absence of electrons. This circumstance is brought about by the screening of the fluctuations of the built-in charge by a charge of opposite sign induced in the metallic electrode of the MIS structure. This screens effectively the fluctuations with scales exceeding the insulator thickness, and the main contribution to the mean squared potential fluctuation is made by charge inhomogeneities of smaller scale. Other differences are due to the quasi-two-dimensional nature of our system.

The effect of random inhomogeneities of the built-in charge on the physical characteristics of MIS were considered also earlier.[4,5,6] There, however, the analysis was restricted to large-scale fluctuations with dimensions greatly exceeding the characteristic lengths of the problem [the thickness of the insulator and the semiconductor space-charge regions (SCR)], and left in fact unanswered the main question, the connection between the parameters of the fluctuation relief of the surface potential and the value of the "built-in charge" and the character of its disposition in the interior of the insulator. This is in fact the subject of the present paper.

A unique feature in our case is some distance between the "built-in" charge and the semiconductor–insulator interface whose potential relief we are investigating. The situation is made complicated by the fact that we have no advance data on the distribution of the built-in charge over the insulator thickness since the experimentally observed quantity—the flat-band voltage V_F—is only integrally connected with the density of the built-in charge even in the simplest case when its density does not depend on the transverse coordinates:

$$V_F=\frac{4\pi}{\varkappa}\int_0^d z\rho(z)\,dz,$$

where $\varkappa$ and d are the dielectric constant and the thickness of the insulator. We consider therefore two hypothetical limiting situations: uniform distribution of the average density of the charged centers over the insulator thickness, and the case when the charged centers are concentrated in a plane at some distance $\lambda<d$ from the interface. If it turns out that the behavior of the experimentally observed quantities differ sufficiently in these cases, then the obtained regularities can turn out to be useful for the explanation of the true position of the built-in charge in real MIS structures.

Another feature of the considered MIS structure is that by varying the voltage on its field electrode it is possible to vary in a wide range the concentration of the mobile carriers on the interface. It is therefore all the more important to ascertain how the fluctuation relief varies as the carriers accumulate in the inversion layer, and also how the fluctuations affect the shape of the volt-capacitance characteristics of the structure. Naturally, we shall also investigate the dependences of the system conductivity on the temperature and on the voltage across the structure.

FORMULATION OF PROBLEM

Consider an MIS structure to whose field electrode is applied a depleting voltage V relative to the superconducting substrate (for the sake of argument, p-type) occupying the half-space $z<0$. The arrangement of the charge centers in a plane parallel to the interface corresponds to a density

$$\frac{1}{e}\rho(z,\mathbf{r})=\delta(\lambda-z)\sigma(\mathbf{r})=\delta(\lambda-z)[\sigma^+(\mathbf{r})-\sigma^-(\mathbf{r})],\qquad(1)$$

where $\mathbf{r}$ is the two-dimensional radius vector in the interface plane, and $\sigma^+(\mathbf{r})$ and $\sigma^-(\mathbf{r})$ are random functions. Assuming the location of the impurity centers to be uncorrelated, we have

$$\langle\sigma(\mathbf{r})\sigma(\mathbf{r}')\rangle-\langle\sigma\rangle^2=\delta(\mathbf{r}-\mathbf{r}')[\langle\sigma^+\rangle+\langle\sigma^-\rangle]\equiv\delta(\mathbf{r}-\mathbf{r}')\sigma,\qquad(2)$$

where $\langle\sigma\rangle$ is the average charge density and $\sigma\equiv\langle\sigma^+\rangle+\langle\sigma^-\rangle$ is the total density of charged centers of both polarities.

The surface potential of the MIS structure is determined by the combined action of the built-in charge, the inversion-layer charge, the charges induced on the metallic electrode, and the ionized acceptors in the depleted region of the substrate. Of importance to us is that this dependence is nonlocal,[1)] and we can write for the surface potential an integral equation, using the Green's function of the corresponding electrostatic problem. The Green's function satisfying the boundary conditions on the electrode and on the space-charge region boundary of the semiconductor, with account taken of the difference between the dielectric constants of the substrate material and the insulator, is quite complicated and unwieldy, but if the doping of the substrate is not strong, so that the specific capacitance of the insulator greatly exceeds the capacitance of the space-charge region (or, in other words, the space-charge region is much thicker than the insulator, the inhomogeneity of the thickness of the depletion region can be neglected. Then

$$\varphi(\mathbf{r})-V=\frac{1}{\varkappa}\int d\mathbf{r}'\int_0^d dz[\rho(\mathbf{r}',z)-e\sigma_e[\varphi(\mathbf{r}')]\delta(z)]\cdot$$
$$\cdot\{[(\mathbf{r}-\mathbf{r}')^2+z^2]^{-1/2}-[(\mathbf{r}-\mathbf{r}')^2+(2d-z)^2]^{-1/2}\},\qquad(3)$$

where $e\sigma[\varphi]$ is the charge of the inversion layer, the dimension of which in the z direction we neglect. The last term in the curly bracket in (3) takes into account the charge induced on the electrode. We note that no allowance is made here for the possible enrichment of the surface by majority carriers, a procedure justified under the condition $\langle\varphi\rangle^2\gg\langle\delta\varphi^2\rangle$ which we shall hereafter assume to be satisfied. In writing down (3) we have also assumed for simplicity that the dielectric constants of the insulator and semiconductor are equal. It will be shown below that this simplification does not

influence the gist of the results. The electron density contained in (3) has an essentially nonlinear dependence on the surface potential and increases strongly when the potential approaches $(\varepsilon_g - \mu)/e$, where ε_g is the width of the forbidden band and μ is the Fermi level in the interior of the semiconductor.

We consider case a situation when the influence of the inversion-layer charge on the surface-potential relief can be neglected. This situation corresponds to small values of the bias V on the structure. The corresponding inequality will be given below. For this case, putting $\sigma_e = 0$ in (3), we easily obtain with the aid of (1) and (2) the mean squared fluctuation of the surface potential:

$$\langle\delta\varphi^2\rangle = 2\pi\sigma\frac{e^2}{\varkappa^2}\int_0 r\,dr[(r^2+\lambda^2)^{-1/2}-(r^2+(2d-\lambda)^2)^{-1/2}]^2$$
$$= 2\pi\sigma\frac{e^2}{\varkappa^2}\ln\left\{\frac{d^2}{(2d-\lambda)\lambda}\right\}. \quad (4)$$

As seen from this expression, in an MIS structure, unlike in three-dimensional systems, the mean squared fluctuation of the potential remains finite even if there are no electrons at all. This is due to the screening of the large-scale fluctuations by the charges induced on the field electrode of the structure. We note also that the amplitude of the fluctuations of the surface potential diverges logarithmically when the charged centers are located directly on the interface with the semiconductor.

ELECTRON SCREENING OF SURFACE-POTENTIAL FLUCTUATIONS. SURFACE STATES

With increasing voltage applied to the structure, the electron concentration in the inversion layer increases. The electrons, now located at the minima of the potential relief, screen the fluctuations of the surface potential. With increasing electron density, the scale of the screened field of the fluctuations of the built-in charge decreases continuously. In fact, consider the inhomogeneities of the built-in charge with some definite scale R, and let the characteristic fluctuations of the charge density in these fluctuations be of the order of $\sigma^{1/2}/R$. If the average electron density σ_e exceeds this value, a negligible spatial redistribution of the electrons suffices to compensate for this inhomogeneity of the built-in charge. For fluctuations having a scale $R \ll \sigma^{1/2}/\sigma_e$ all the electrons are at the minima of the potential, and the electron charge density is much less than the excess charge of the fluctuations. The potential of such small-scale fluctuations is therefore in fact unscreened. Consequently, at a given average electron density σ_e, when calculating the amplitude of the potential fluctuations, it is necessary to take into account only the fluctuations of the built-in charge with scale less than $\sigma^{1/2}/\sigma_e$, i.e., substitute this quantity as the upper limit of integration in (4), which additively takes into account the contributions of fluctuations of all scales.[2)] It turns out that at low concentrations $\sigma_e \ll \sigma^{1/2}/d$ the presence of the electrons has practically no effect on the amplitude of the potential fluctuations, and this amplitude is given as before by expression (4). This result should have been expected, for at such low concentrations the electrons smooth out the inhomogeneities of a built-in charge with a scale greatly exceeding the thickness of the insulator, and even without this smoothing the inhomogeneities are well screened by the charges induced on the electrode. If the inverse inequality holds, we have

$$\langle\delta\varphi^2\rangle = \delta\varphi_0^2\ln(\sigma^{1/2}/\lambda\sigma_e),\quad \delta\varphi_0^2 = 2\pi\sigma e^2/\varkappa^2, \quad (5)$$

or

$$\sigma_e = \sigma^{1/2}\lambda^{-1}\exp\{-\langle\delta\varphi^2\rangle/\delta\varphi_0^2\}, \quad (6)$$

i.e., the square of the amplitude of the fluctuations of the potential decreases logarithmically with increasing average concentration of the electrons.

At small λ, however, it must be recognized that the energy of the electron differs, on account of the quantum correction necessitated by the localization of its transverse motion, from the potential energy at the interface and consequently does not become infinite as $\lambda \to 0$. We estimate a typical value of the distance z_0 of the electron from the surface by minimizing the expression for the total energy of the electron:

$$\frac{\hbar^2}{2mz_0^2} - \frac{\sigma^{1/2}e^2}{\varkappa}\ln^{1/2}\frac{\sigma^{1/2}}{(\lambda+z_0)\sigma_e}, \quad (7)$$

where the role of potential energy is now taken by the dependence of the average depth of the fluctuation minimum on the distance into the interior of the semiconductor. We obtain $z_0 \approx (a^2/\sigma)^{1/4}$ at $\lambda \ll (a^2/\sigma)^{1/4}$, where $a = \hbar^2\varkappa/me^2$ is the Bohr radius, and $z_0 \approx (a\lambda/\sigma^{1/2})^{1/3}$ if the inverse condition is satisfied. In the latter case the localization energy can be disregarded. At small λ, the average depth of the minimum of the electron energy is equal to

$$\frac{e^2}{\varkappa}\sigma^{1/2}\ln^{1/2}\frac{\sigma^{3/4}}{\sigma_e a^{1/2}}. \quad (8)$$

To find the conduction activation energy, as well as the connection between the average electron concentration and the average surface potential, we must determine the dependence of the position of the Fermi level on the surface on the average surface concentration of the electrons. We consider to this end the spatial distribution of the electrons in fluctuations with critical radius $R_c = \sigma^{1/2}/\sigma_e$ and introduce in succession, just as in Refs. 3 and 7, fluctuations of scale that decreases continuously compared with R_c, assuming that the charged-center concentration is $\sigma \gg a^{-2}$. Since the excess charge concentration for fluctuations of scale $R \ll R_c$ is $\sigma^{1/2}/R \gg \sigma_e$, the electrons will occupy only a small fraction of "bins" of this dimension, in which the potential is successively decreased by the fluctuations of all scales larger than R. This "crumbling" process is limited by quantum effects, namely by the circumstance that at sufficiently small fluctuations the number of quantum levels in the corresponding potential well is of the order of the excess charge in it. From this condition we get the limiting dimension of the electron "drops", by equating the number of states $R^2k_{\max}^2$ to the excess charge $R\sigma^{1/2}$, and the Fermi energy

$$\frac{\hbar^2k_{max}^2}{2m} = \frac{e^2}{\varkappa}\sigma^{1/2}\ln^{1/2}\frac{R\sigma^{1/4}}{a^{1/2}} \quad (9)$$

to the characteristic value of the potential energy of the electron in the fluctuation with dimension R. We obtain

$R \approx a$. We have assumed here a two-dimensional state density, since at $\lambda < (a^2/\sigma)^{1/4}$ the "quantum" of energy of transverse motion turns out to be of the order of the depth of the well. In this case, a potential minimum of critical radius R_c contains on the average R_c/a electron drops distributed with a density $\sigma_e(\sigma a^2)^{-1/2}$, while each drop contains $a\sigma^{1/2} \gg 1$ electrons. With increasing electron density, the concentration of the drops increases while the number of electrons in each drop remains the same. Nor does the position of the Fermi level change relative to the bottom of the potential minima:

$$\Delta \approx \varkappa^{-1} e^2 \sigma^{1/2} \ln^{1/2} (a^2\sigma)^{1/4}.$$

At $\sigma_e \ll \sigma^{1/2}/s$ this energy is small compared with the total depth of the potential well ($\Delta^2 \ll \langle \delta\varphi^2 \rangle$), and the Fermi energy should be of the order of the mean squared amplitude of the fluctuations, i.e.,

$$\langle E_c \rangle - E_F = \gamma \frac{e^2}{\varkappa} \sigma^{1/2} \ln^{1/2} \frac{\sigma^{3/4}}{\sigma_e a^{1/2}}, \tag{10}$$

where γ is a coefficient of the order of unity. Therefore equating the position of the Fermi level in the semiconductor volume and on the surface, we obtain the average bending of the bands $\langle \varphi \rangle$, corresponding to a definite value of the average electron concentration σ_e

$$\langle \varphi \rangle = \varepsilon_g - \mu - \gamma \frac{e^2}{\varkappa} \sigma^{1/2} \ln^{1/2} \frac{\sigma^{3/4}}{\sigma_e a^{1/2}}. \tag{11}$$

If the distance from the built-in charge and the interface exceeds the Bohr radius, $\lambda \gg a$, a condition corresponding to (9) yields a drop dimension $R \approx \lambda$ and a Fermi energy

$$\Delta \approx \frac{\hbar^2}{2m} \frac{\sigma^{1/2}}{\lambda} \ll \frac{e^2}{\varkappa} \sigma^{1/2}.$$

Then

$$\langle E_c \rangle - E_F = \gamma \frac{e^2}{\varkappa} (2\pi\sigma)^{1/2} \ln^{1/2} \frac{\sigma^{1/2}}{\sigma_e \lambda}. \tag{12}$$

At the same time, formulas (10) and (12) yield the average electron charge on the surface as a function of the average band bending. Its value greatly exceeds the charge of the inversion layer in a homogeneous MIS structure at the same value of the surface potential. The additional voltage drop on the insulator, due to this charge, deforms the $C-V$ characteristics of the MIS structure compared with the ideal ones, precisely in the same manner as on account of the surface states in the forbidden band of a semiconductor. It is quite probable that in some energy band the surface-state density N_{SS} determined from $C-V$ measurements is governed precisely by these fluctuations of the surface potential. The state density corresponding to the fluctuations is obtained by differentiating σ_e from (10) and (12) with respect to energy. At $\lambda \gg a$ we obtain

$$N_{ss}(\varepsilon) = \frac{d\sigma_e}{dE_F} = \frac{\sigma^{1/2}}{\lambda} \frac{2\varepsilon}{\gamma^2 e^2 \delta\varphi_0^2} \exp\left\{ -\frac{\varepsilon^2}{\gamma^2 e^2 \delta\varphi_0^2} \right\}, \tag{13}$$

where $\delta\varphi_0^2 = 2\pi\sigma e^2/\varkappa^2$, and ε is the energy reckoned from the conduction band into the interior of the forbidden band. At $\lambda \ll a$ it is necessary to replace λ in (13) by $(a^2/\sigma)^{1/4}$. Attention is called to the fact that according to (13) N_{SS} has a maximum $N_{SS}^{\max} \approx \varkappa/\lambda e^2$ at $\varepsilon = \gamma e(\delta\varphi_0^2/2)^{1/2}$, and this corresponds to a total concentration $\sigma_e \approx \sigma^{1/2}/\lambda$, when the critical radius R_c becomes of the order of the drop dimension λ and the drops begin to merge with one another. In this region, the fluctuation amplitude depends so strongly on the electron density that the derivative $2\sigma_e/\sigma\langle\delta\varphi^2\rangle^{1/2}$ decreases with decreasing $\langle\delta\varphi^2\rangle$. It must be noted, however, that one can speak with full certainty of a maximum of N_{SS} only if $\lambda \gg a$, for when $\lambda \ll a$ the energy of the maximum of N_{SS} is of the same order as our uncertainty in the determination of the Fermi level Δ.

Expression (13) for the effective density of the surface states due to the fluctuations is valid only near the conduction band, when $\varepsilon^2 < e^2\delta\varphi_0^2 \ln(d/\lambda)$, and $\sigma_e > \sigma^{1/2}/d$, i.e., if the fluctuation amplitude depends substantially on the electron density. At lower electron concentration, as we already know, the amplitude of the fluctuations is practically independent of σ_e and the electrons are located only in surface sections that are quite far from one another and in which the depth of the potential minima greatly exceeds the average depth. Let, for example, in some such section the potential $e\varphi$ produced by the impurities turn out to be less than the Fermi level. Inasmuch as at low electron concentration the characteristic length over which the potential varies is equal to the insulator thickness, the area of this section is of the order d^2. Consequently, to raise here the potential to the Fermi level it is necessary to have a compensating electron charge $e^{-2}\varkappa d(e\delta\varphi + E_F - \langle E_c \rangle)$. In our problem ($\sigma a^2 \gg 1$), the fluctuation potential is due mainly to Gaussian impurity-charge fluctuations that contain many particles. The potential distribution function is therefore also Gaussian, with a variance $\langle\delta\varphi^2\rangle$, determined by expression (4). The average electron concentration is then

$$\sigma_e = \frac{\varkappa}{e^2 d} \int_{\langle E_c \rangle - E_F}^{\infty} \frac{d\varphi}{(\pi\langle\delta\varphi^2\rangle)^{1/2}} (e\delta\varphi + E_F - \langle E_c \rangle) \exp\{-\delta\varphi^2/\langle\delta\varphi^2\rangle\}. \tag{14}$$

Differentiating with respect to E_F and again putting $\langle E_c \rangle - E_F = \varepsilon$, we obtain

$$N_{ss} = \frac{\varkappa}{e^2 d} \Phi\left\{ \frac{\varepsilon}{\langle\delta\varphi^2\rangle^{1/2}} \right\}, \tag{15}$$

where Φ is the error function. The region of validity of this expression is $\varepsilon^2 \ll \langle\delta\varphi^2\rangle$.

Figure 2 (curve 1) shows in units of $\varkappa/e^2 d$ and $e^2\sigma^{1/2}/\varkappa$ the energy dependence of the effective state density N_{SS}, corresponding to localization of the built-in charge in a plane $\lambda = 0.1d$. By way of estimate we put[3)] $\sigma = 10^{12}$ cm^{-2}, $d = 10^{-5}$ cm, $\gamma = 1$, and $\varkappa = 8$; the characteristic energy is then $e^2\sigma^{1/2}/\varkappa \approx 2 \times 10^{-2}$ eV and $N_{SS}^{\max} \approx 2 \times 10^{13}$ cm^{-2} eV^{-1}.

We turn now to the investigation of a situation when

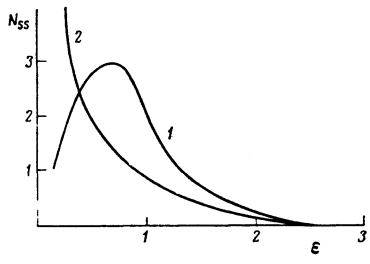

FIG. 2.

the built-in charge is "smeared" out in the interior of the insulator. At a low electron concentration $\sigma_e < \sigma^{1/2}/d$ the mean squared fluctuation of the potential can be easily obtained by averaging (4) over λ:

$$\langle\delta\varphi^2\rangle = 4\pi\sigma\frac{e^2}{\varkappa^2}(1-\ln 2). \tag{16}$$

If the concentration of the electrons is high, and we calculate the mean squared fluctuation of a surface potential with critical scale R_c smaller than the insulator thickness d, we must, limiting in (4) the region of integration with respect to r, restrict to the same value R_c also the region of averaging over $\lambda(0<\lambda<R_c)$, since the contribution made to the surface potential by the small-scale charge fluctuations located farther than R_c from the interface are effectively averaged out. The dependence of the mean squared amplitude of the potential on the fluctuation radius turns out then to be the same as in the three-dimensional case:

$$\langle\delta\varphi^2\rangle = 2\pi\frac{e^2}{\varkappa^2}\frac{\sigma}{d}R_c, \tag{17}$$

where σ/d is the exchange density of the charged centers. We obtain the critical radius by equating the electron charge $\sigma_e R_c^2$ to the excess charge $\sigma d^{-1}R_c^3)^{1/2}$ in the volume R_c^3, whence $R_c = \sigma/d\sigma_e^2$ and

$$\langle\delta\varphi^2\rangle = 2\pi\frac{e^2}{\varkappa^2}\left(\frac{\sigma}{\sigma_e}\frac{1}{d}\right)^2. \tag{18}$$

Thus, for a "smeared" built-in charge the amplitude of the fluctuations decreases at $\sigma_e > \sigma^{1/2}/d$ in inverse proportion to σ_e, as against the logarithmic dependence in the case of a charge localized in a plane. Just as before, to determine the position of the Fermi level we consider in succession fluctuations with ever increasing scale compared with R_c. The dimension of the electron drops, in which the number of quantum levels is of the order of the excess charge, turns out to be of the order of the Bohr radius a, and the corresponding Fermi energy is $(e^2/\varkappa)(\sigma a/d)^{1/2} = \varepsilon_0(\sigma a^3/d)^{1/2}$. These estimates are valid when the drop contains many levels, i.e., when the condition $(\sigma/d)a^3 \gg 1$ is satisfied, a condition that cannot be regarded as realistic enough in the case, e.g., of Si-SiO_2 structures. In the opposite case, the "crumbling" procedure must be stopped with the dimension $(\sigma/d)^{-1/2}$, which corresponds to the average distance between the charged centers. In this case the electrons that screen the potential of a fluctuation of critical radius R_c will individually be located on the interface near certain positive centers, in whose vicinity the potential energy is successively decreased by fluctuations with scales $R_c > R > (\sigma/d)^{-1/3}$.

Since such a center is located on the average at a distance $(d/\sigma)^{1/3} \gg a$ away from the boundary, the quantum correction to the electron energy is small compared with the Coulomb correction, and the Fermi level can be regarded as passing directly over the bottom of the well. Consequently $\langle E_c\rangle - E_F = \gamma\langle\delta\varphi^2\rangle^{1/2}$ at a given σ_e, where $\langle\delta\varphi^2\rangle$ is determined by expression (18). Differentiating σ_e from (18) with respect to energy, we obtain the effective state density

$$N_{ss}(\varepsilon) = \sigma\frac{e^2}{\varkappa d}\frac{1}{\varepsilon^2}. \tag{19}$$

This formula is valid at $\varepsilon < e^2\sigma^{1/2}/\varkappa$. It is clear that at high energies $N_{ss}(\varepsilon)$ is determined by formula (15) with variance (16). The form of $N_{ss}(\varepsilon)$ for a "smeared" built-in charge is shown in Fig. 2 (curve 2).

It remains for us only to consider the situation that arises at low density of the built-in charge $\sigma a^2 \ll 1$, concentrated in a plane close to the interface, $\lambda \ll a$ (we put henceforth $\lambda = 0$). We note first that if the condition $\sigma a^2 \ll 1$ is satisfied the wave functions of the bound states, which undoubtedly exist on positive centers, do not overlap in practice, and their binding energy $\varepsilon_0(\varepsilon_0 = e^2/8\varkappa a$ in the simplest case without allowance for the anisotropy of the effective mass) greatly exceeds the characteristic energy of the fluctuations. It is these states which are first filled with electrons as the voltage on the structure increases.

The small-scale fluctuations, i.e., the presence of another center (positive or negative) near the considered positive center, at a distance R much less than the average $\sigma^{-1/2}$ but larger than a, leads to a shift of the binding energy by an amount $\pm e^2/\varkappa R$. At low electron density, $\sigma_e \ll \sigma^+$, the states filled are those with energy lowered because of the proximity to the other positive center. The probability of an approach that ensures an energy shift $\varepsilon - \varepsilon_0 = e^2/\varkappa R$ is given by

$$(\sigma^+)^2\pi R\,dR = (\sigma^+)^2\pi\frac{e^4}{\varkappa^2}\frac{d\varepsilon}{(\varepsilon-\varepsilon_0)^3} = N_{ss}(\varepsilon)\,d\varepsilon. \tag{20}$$

At a given value of the Fermi level, all the states with lower energy will be filled. Therefore, integrating (2) up to $E_F = \varepsilon_g - \mu - e\langle\varphi\rangle$, we obtain the electron concentration corresponding to the given value of the average surface potential $\langle\varphi\rangle$:

$$\sigma_e = (\sigma^+)^2\frac{\pi}{2}\frac{e^4}{\varkappa^2}\frac{1}{(\varepsilon_g-\mu-e\langle\varphi\rangle-\varepsilon_0)^2}. \tag{21}$$

Expressions (20) and (21) are valid at $\sigma_e \ll \sigma^+$, while $\varepsilon_g - \mu - e\langle\varphi\rangle - \varepsilon_0 \gg e^2\sigma^{1/2}/\varkappa$, i.e., for deep fluctuations that can be regarded, with enough justification, as paired. The multi-electron character of the problem prevents us from tracing the state density in the immediate vicinity of the level ε_0. At $\sigma - \sigma_e \ll \sigma^+$, however, we can in exactly the same way find the shape of the oppositely located "trail" due to the interaction with the close repelling centers:

$$N_{ss}(\varepsilon) = \sigma^+\sigma^-\pi\frac{e^4}{\varkappa^2}\frac{1}{(\varepsilon_0-\varepsilon)^3}. \tag{22}$$

It is clear that the integral number of states in this peak is equal to σ^+. We note that in the considered two-dimensional system, owing to the high probability of the mutual approach of neighboring atoms, the fluctuation broadening of the bound state whose wings are

described by (20) and (22) turns out to be larger than in three-dimensional systems.[3] We note also that the depth of the level ε_0 need not necessarily be determined by a hydrogenlike expression, i.e., the level itself may, for a variety of reasons, be also "deep", but our expressions (20) and (22) for the state-density "tails" due to the Coulomb interaction of the neighboring atoms will remain in force.

After the bound states on the positive centers are filled, further increase of the electron density takes place against the background of the potential relief produced exclusively by negatively charged repelling centers. The minima of the potential energy correspond then to rarefactions in the spatial distribution of the repelling centers. To obtain the measured fluctuation of the potential in this case, it is necessary to replace in expression (5) σ by σ^- and λ by $(\sigma^-)^{-1/2}$, since shorter-wave components of (4) correspond to the square of the potential of an individual atom and not to potential-relief fluctuations due to fluctuations in the relative positions of the atoms. Then

$$\langle\delta\varphi^2\rangle=2\pi\frac{e^2}{\varkappa^2}\sigma^-\ln\frac{\sigma^-}{\sigma_e}, \tag{23}$$

and

$$N_{ss}=\frac{\varkappa^2\varepsilon}{\pi e^4}\exp\left\{-\frac{\varkappa^2\varepsilon^2}{2\pi e^4\sigma^-}\right\}. \tag{24}$$

These expressions are valid if $\sigma_e \ll \sigma^-$, for when $\sigma_e \sim \sigma^-$ the actual scale R_c of the fluctuations is of the order of the average distance between the repelling centers. For such non-Gaussian fluctuations that contain on the average one center , the employed concept of nonlinear screening and the corresponding expression for $R_c = \sigma^{1/2}/\sigma_e$, becomes meaningless. Expression (23) is incorrect also deep enough in the forbidden band at

$$\varepsilon > \frac{e^2}{\varkappa}(\sigma^-)^{1/2}\ln^{1/2}(d(\sigma^-)^{1/2}),$$

but is less than ε_0. It is necessary here to use formula (17) with the corresponding value of the mean squared fluctuation of the potential. It must be emphasized that the main singularity of the considered situation with $\lambda=0$ and $\sigma a^2 \ll 1$ is the peak of the density in the depth of the band, a peak due to the bound state ε_0.

Let us summarize briefly our results. The main conclusion of our investigation is that the fluctuation relief of the surface potential in MIS structure is essentially small-scale. In fact, its mean squared amplitude is close to the potential of an individual impurity over a length corresponding to the average distance between the impurity atoms, and depends very weakly (logarithmically) on the fluctuation scale. This behavior is due to the two-dimensional character of our system, where the mean squared fluctuations of the charge increase with the fluctuation scale more slowly than in the three-dimensional case. Therefore the mean squared fluctuation of the potential responds weakly to the character of the distribution of the built-in charge in the interior of the insulator and is practically independent of the electron density all the way to the limiting concentrations that correspond (at small σ) to an electron for each impurity atom. Since fluctuations of such small scale are not Gaussian, our expressions, obtained by starting with the "large scale" premises, are not valid for this region. Where our results are correct enough, i.e., at small σ_e, the amplitude of the fluctuations varies exceedingly weakly. The only exception is the case when $\lambda \gg a$ and $\sigma\lambda^2 \gg 1$, when the potential of fluctuations with $R<\lambda$ increases steeply with the radius, the quantum effects are small, and the actual fluctuations with $R\sim\lambda$ contain a sufficiently large number of particles. It is only here that it is possible to trace correctly the dependence of $\langle\delta\varphi^2\rangle$ on the electron density in almost the entire range of variation of the fluctuation amplitude with change of the electron concentration.

SURFACE CONDUCTIVITY

The conductivity of carriers situated in a random potential field has been sufficiently well investigated[7] and it is not particularly difficult to apply these results to our case. It is known that the conductivity is determined by two competing mechanisms—activation hopping of the electrons from one minimum of the potential to another, and tunneling of the carriers between these minima. In the former case the electron should acquire from the thermostat (the crystal lattice) an additional energy $E_p - E_F \sim \langle\delta\varphi^2\rangle^{1/2}$, where E_p is the "percolation level"—the average energy of the saddle points that separate the minima of the potential; therefore the probability of such a process is proportional to $\exp\{-\langle\delta\varphi^2\rangle^{1/2}T\}$ (here T is the temperature in energy units). The tunneling probability depends substantially also on the scale of the potential relief $\exp\{-2\hbar^{-1}R_c \times (m^2\langle\delta\phi^2\rangle^{1/4}$. Comparing the argument of the exponential, we estimate the temperature at which the transition from the activation conductivity to the tunneling conductivity takes place:

$$(T_0)^2 \approx \frac{\hbar^2}{2m}\frac{e^2}{\varkappa}\frac{\sigma_e^2}{\sigma^{1/2}}\ln^{1/2}\frac{\sigma^{1/2}}{\lambda\sigma_e} \tag{25}$$

for a built-in charge localized in the plane λ, and

$$(T_0) \approx \frac{\hbar^2}{2m}\frac{e^2}{\varkappa}\frac{\sigma_e^3}{\sigma}d$$

for the case of a "smeared" charge. At $T>T_0$ the surface conductivity is of the activation type with a characteristic energy of order $\langle\delta\varphi^2\rangle^{1/2}$, and at lower temperatures the conductivity is of the tunnel type. However, even at $T<T_0$ the conductivity can depend exponentially on the temperature, but with a much lower activation energy. The point is that when the conditions $\sigma a^2 \gg 1$ and $\sigma\lambda^2 \gg 1$ are satisfied the electrons, as we have seen, are localized in the form of "quantum drops" in minima with scale R_c. In these drops the distance between levels, near the Fermi level, is of

the order of

$$\frac{\hbar^2}{m}k_m\Delta k \approx \frac{\hbar^2}{m\lambda^2}(\sigma\lambda^2)^{1/4}=\Delta', \tag{26}$$

for example, for the case $\lambda \gg a$. Recognizing that the energy position of the bottom of these drops is random, we can conclude that the energy shift between the upper occupied level in one of the drops and a lower free level in another drop belonging to another R_c minimum is of the order Δ'. Therefore at $T<\Delta'$ the tunnel conductivity is proportional to $\exp\{-\Delta'/T\}$. At very low temperatures, however, it may turn out that it is easier for the electron to tunnel through a distance somewhat larger than between nearest drops of neighboring R_c minimum, and find thereby a drop with a more suitable energy of the lower free level. The increase of the tunneling path R decreases the transition probability by a factor $\exp\{-\hbar^{-1}R(m^2\langle\delta\phi^2\rangle)^{1/4}\}$. On the other hand, the electron can reach in this case $n=R^2/R_c\lambda$ drops and choose from among them the drop with a smallest energy difference on the order of Δ'/n. By determining the maximum of the expression

$$\exp\left\{-\frac{R}{\hbar}\left(m^2\frac{e^4}{\varkappa^2}\sigma\right)^{1/4}-\frac{1}{T}\frac{\hbar^2}{m\lambda}\frac{R_c}{R^2}(\sigma\lambda^2)^{1/4}\right\},$$

we obtain a conductivity with a temperature dependence

$$\exp\{-(T_c/T)^{1/4}\}, \tag{27}$$

which is sometimes called, just as the $\exp\{-T_c/T)^{1/4}\}$ dependence, Mott's law. Here

$$T_c \approx \frac{\hbar^2}{ma\lambda}\frac{\sigma}{\sigma_e}(\sigma\lambda^2)^{1/4};$$

this temperature decreases with increasing electron density. The region of applicability of this expression is

$$T<\frac{\hbar^2}{m\lambda^2}\left(\frac{\sigma_e}{\sigma^{1/2}}a\right)^{1/2}<\Delta'.$$

It must be stated that by now there are in the literature several reports of experimental observation of a surface-conductivity temperature dependence similar to (17) (see e.g., Ref. 8). The surface conductivity is measured on MIS-structure transistors at low voltages between the source and the drain. Under such a quasi-equilibrium situation the chemical potential in the bulk of the semiconductor is practically the same as on the surface. In MIS devices of the SCR type one encounters also another situation, wherein nonequilibrium surface charge with some initial distribution flows down either under another electrode with a large potential, or into the drain junction. The macroscopic tangential surface electric field due to the electrostatic-repulsion forces is then given by $\varepsilon=\text{grad}\{4\pi e\,\varkappa^{-1}d\sigma_e\}$. The surface conductivity by which the electric field must be multiplied to obtain the current is either proportional to σ_e if σ_e exceeds the integral surface-state density σ_0 due to the fluctuations (in the situations considered by us $\sigma_0 \approx \{\sigma, \sigma^{1/2}/\lambda, (\sigma/d)^{2/3}, \sigma/(\sigma a^2)^{1/4})$, or is proportional to the quantity

$$\frac{mT}{\pi\hbar^2}\exp\left\{-\frac{\langle\delta\varphi^2\rangle^{1/2}}{T}\right\}$$

at $\sigma_e<\sigma_0$, when the fluctuations are not screens. The current is then substituted in the continuity equation. It turns out that the final charge-flow stage $\sigma_e<\sigma_0$ is described by a linear diffusion equation with an effective diffusion coefficient

$$D^*=D\frac{d}{a}\exp\left\{-\frac{\langle\delta\varphi^2\rangle^{1/2}}{T}\right\}.$$

Here D is the ordinary diffusion coefficient. At a known electrode geometry we can easily calculate the losses due to the fact that the charge does not manage to flow from under one electrode to another during the timing pulse, and by measuring these losses at various temperatures and frequency, we can determine the characteristic amplitude of the fluctuations and the integral density of states due to the fluctuations.

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[1)]The customarily employed local relation between the surface potential and the charge density, in terms of the specific capacitances, is valid only when the characteristic dimension of the inhomogeneities is much larger than the thicknesses of the dielectric and of the space-charge region.

[2)]The arguments used by us concerning the character of the nonlinear electronic screening were first advanced by Shklovskiĭ and Éfros[2, 3] as applied to three-dimensional systems.

[3)]As we have seen, the main contribution to the amplitude of the potential fluctuations is made by small-scale fluctuations of the built-in charge with dimension smaller than d. Analysis shows that for such small-scale fluctuations allowance for the difference between the dielectric constants of the semiconductor and of the insulator makes it necessary to assume $\varkappa$ in all expression to be equal to the effective dielectric constant $(\varkappa_1+\varkappa_2)/2$.

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