Influence of the Coulomb interaction on the spectrum of surface states of a semiconductor with different degrees of occupancy

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An analysis is made of the influence of the Coulomb interaction on the spectrum of monoenergetic donor centers located on the surface of a semiconductor. It is shown that the main contribution to the dispersion of the potential is made by a small-scale potential with a characteristic size of the order of the average distance between charges. The energy distribution of the donor centers is calculated as a function of their degree of occupancy. At low concentrations of charged centers there is a gap between the empty and filled states and this gap disappears on increase in the charge concentration. The presence of this gap in the density of states is a consequence of ordering of charged donors, i.e., of the Wigner crystallization. Elementary excitations are considered under the Wigner crystallization conditions. The dependences of the concentration of charged donors, of the bending of the semiconductor bands, and of the capacitance on the external voltage are determined for a metal–insulator–semiconductor structure. The band bending is found to be a continuous function of the voltage and the capacitance diverges as the concentration of charged centers tends to zero.

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1. INTRODUCTION

A characteristic property of a semiconductor–insulator (SI) interface is the presence of surface centers. The Coulomb interactions between charged centers creates an inhomogeneous fluctuation potential in the plane of the interface and this results in a smearing of the energy of the surface centers. This fluctuation potential is responsible for such characteristics of the observed quantities as the frequency dependence of the capacitance and resistance of metal–insulator–semiconductor (MIS) structures[1,2] and the dependence of the longitudinal conductance along the SI interface on the external field.[3,4]

It has been suggested on several occasions[1,5,6] that such charge inhomogeneities are of the large-scale type. However, the two-dimensional nature of the charge distribution on an SI interface has the effect that the main contribution to fluctuations depending on the semiconductor bands is made by small-scale fluctuations of the charge.[7,8] Gergel' and Suris[8] analyzed this aspect in detail and found a relationship between dispersion of the charge and dispersion of the potential, considered as a function of the density of free electrons in the surface region of the semiconductor.

It is assumed in Refs. 1 and 5–8 that the fluctuating charge is frozen-in (built in) and it is screened solely by free carriers in the metal and also in the semiconductor near the SI interface. This can be assumed only if these states are separated by a large gap from the Fermi level. We shall consider the situation when the energies of the surface states are in the band gap of the semiconductor. Consequently, their charge state is governed by the position of the Fermi level and varies with the bending of the semiconductor bands. On the other hand, the existence of a charge on the Si interface results in smearing of the energies of the surface states and this in turn affects their charge. Thus, allowance for the Coulomb interaction on the occupancy of the surface states in the case of changes in the bending of the semiconductor bands requires self-consistency.

The potential at an SI interface is inhomogeneous by its very nature because of the discrete distribution of the charge on the surface and also because of the fluctuations of this distribution on the interface. Such an inhomogeneous (fluctuation) potential depends strongly on the nature of the screening of the charge. This screening is due to a redistribution of the charge in the metal and semiconductor, and between the surface states. In the case when the surface states are partly filled, the most important effect is the screening of the fluctuation potential because of a redistribution of the charge between the surface states, since in the limiting cases of completely empty donor states or completely filled gaps we have the built-in charge situation discussed in Refs. 1 and 5–8.

We shall calculate the self-consistent fluctuation potential as a function of the degree of occupancy of the surface states and also find the influence of the fluctuation potential on the density of states of the surface centers, on their occupancy considered as a function of the external voltage applied to an MIS structure, and on the capacitance of such a structure.

2. POTENTIAL AT A SEMICONDUCTOR–INSULATOR INTERFACE

We shall consider an MIS structure with a p-type semiconductor doped with shallow acceptors (concentration N_a) and donor surface states distributed at random over the SI interface. We shall assume that the surface donor level is monoenergetic with an energy E_0, concentration σ, and wave function radius a. We shall confine our analysis to the light doping case when $\sigma a^2 \ll 1$.

Under a sufficiently strong depletion voltage on an MIS structure (corresponding to a strong band bending on the semicondcutor surface) the donors are under the Fermi level and are consequently neutral. The energy band scheme of an MIS structure is shown in Fig. 1. In this case the density of the donor states is a delta-like peak. Reduction in the band bending of the semiconductor results in the onset of the donor ionization and creates an inhomogeneous potential in the plane of the SI interface. The presence of this inhomogeneous potential smears the energies of the donor centers. The nature of smearing and, consequently, the density of the surface states are governed by the charged donor concentration σ_+, and the value of σ_+ itself depends on the number of states located above the Fermi level.

The local value of the potential energy on the surface of a semiconductor at an arbitrary point r can be represented by a sum of the energies created by the donor charge (concentration σ_+) on the SI interface, the charge on the metal (surface concentration σ_m), and space charge of the semiconductor.

The appearance of the charge on the surface redistributes the charges in the metal and semiconductor. The screening by the bulk of the semiconductor is nonlinear. In the MIS structure under consideration the semiconductor has a Schottky depletion layer of thickness L and a charge density $\rho=-qN_a$. The screening in the semiconductor is due to a change in the thickness of this layer by ΔL. We can show that in the case of small thicknesses of the insulator d

$$d/L \ll N_a L^3$$

the change in the thickness of the Schottky layer due to the screening of the charge fluctuations is considerably less than the thickness itself[1)] ($\Delta L \ll L$). In this case we can assume there is a metal electrode at the boundary of the Schottky layer located at a depth L from the semiconductor surface.[7] The screening in the semiconductor is then linear and the potential can be regarded as a sum of the potentials due to the charges on the surface and of their image forces in the metal and semiconductor.

The potential at an arbitrary point $\mathbf{r}$ on the semiconductor surface can be written in the form

$$V(\mathbf{r})=B+\sum_i v(\mathbf{r}-\mathbf{r}_i), \tag{1}$$

where B is a potential created by the homogeneous part of the charge located in the metal and in the semiconductor, and $v(\mathbf{r}-\mathbf{r}_i)$ is the potential of a charged donor located on the surface at a point $\mathbf{r}_i$ when allowance is made for its image forces in the metal and semiconductor.

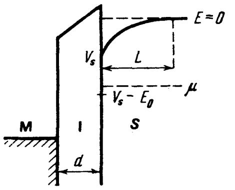

FIG. 1. Energy band scheme of an MIS structure subjected to an external voltage.

We shall find expressions for $v(\mathbf{r}-\mathbf{r}_i)$ and the constant B. Point charges on the SI interface will be expanded into Fourier harmonics in the plane of this interface: $\sigma_k=q/(2\pi)^2$. The potential created by a charge harmonic σ_k, subject to allowance for the boundary conditions, is

$$V_k=-\frac{4_i\, q\sigma_s}{k(\varepsilon_i \operatorname{cth} kd+\varepsilon_s \operatorname{cth} kL)}, \tag{2}$$

where ε_i and ε_s are the permittivities of the insulator and semiconductor, respectively. Inverse Fourier transformation gives the potential created by the point charge:

$$v(\mathbf{r}-\mathbf{r}_i)=-2q^2\int_0 \frac{J_0(k|\mathbf{r}-\mathbf{r}_i|)\,dk}{\varepsilon_i \operatorname{cth} kd+\varepsilon_s \operatorname{cth} kL}, \tag{3}$$

where $J_0(x)$ is a Bessel function of zeroth order.

It follows from the definition of the average potential

$$\bar{V}(\mathbf{r})=\lim\frac{1}{\pi R^2}\int V(\mathbf{r})\,d\mathbf{r},$$

which will be denoted by V_s, and also from Eqs. (1) and (3), that

$$B=V_s-B_1,$$

where B_1 is found from the expression

$$B_1=-\lim\frac{2q^2}{\pi R^2}\int_0^R r\,dr\sum_{i=1}^N\int_0^{2\pi} d\varphi_i\int_0^\infty \frac{J_0(k|\mathbf{r}-\mathbf{r}_i|)\,dk}{\varepsilon_i \operatorname{cth} kd+\varepsilon_s \operatorname{cth} kL}. \tag{4}$$

Here, φ_i is the angle between the vectors $\mathbf{r}$ and $\mathbf{r}_i$, and the summation is carried out over all the charged centers in a circle of radius R. Calculations showed that Eq. (4) gives

$$B_1=-4\pi q^2\sigma_+ d/\varepsilon_1, \quad \varepsilon_1=\varepsilon_i+d\varepsilon_s/L. \tag{5}$$

The constant B_1 is the average potential at the SI interface created solely by the charged donors whose concentration is σ_+. In fact, it is the zeroth harmonic of the potential which can be found from Eq. (2) by allowing k to approach zero and assuming that $\sigma_{k=0}=\sigma_+$.

If zero potential is taken in the bulk of the semiconductor, the value of V_s is given by the familiar expression

$$V_s=-2\pi q^2 N_a L^2/\varepsilon_s. \tag{6}$$

We have thus determined completely the quantity B in Eqs. (1).

3. SMALL-SCALE POTENTIAL AND FERMI LEVEL

The energy of an electron at a donor located at a point $\mathbf{r}$ is given by

$$E(\mathbf{r})=-E_0+V(\mathbf{r}). \tag{7}$$

It has been pointed out earlier[7,8] that the main contribution to the dispersion of the fluctuation potential is made by small-scale fluctuations of size smaller than the average distance between the charge amounting to $(\pi\sigma_+)^{-1/2}$. As the first approximation in the expression (1) for the potential at some point we shall include exactly the potential of the nearest charged center located at a distance r from the point in question, and we shall average the potentials of all the remaining charges over their positions on the surface. Later (Sec. 6) we shall discuss the limits of validity of this approximation. In the averaging process we have to allow for the correlation in the distribution of the charged donors. Since as a result of the above averaging the energy of a donor center is a regular and monotonic function of the distance r, i.e., $E(r)$, we can introduce the concept of the Fermi radius r_F, defined by

$$E(r_F)=-E_0+V(r_F)=\mu, \tag{8}$$

where μ is the position of the Fermi level in the bulk of the semiconductor. It follows from this definition that all the donors located at distances smaller than r_F from the charged donor are neutral.

Thus, in the calculation of the potential at a point located at a distance r from the nearest charged donor the averaging over all the remaining charges should be made in the region outside a circle of radius r_F centered at the point of position of the nearest charged donor. Consequently, the potential at a distance r from the nearest charged donor is

$$V(r)=V_s+v(r)+V_c(r,\ r_F), \tag{9}$$

where $v(r)$ is given by Eq. (3) and $V_c(r, r_F)$ is

$$V_c(r,r_F)=\begin{cases} 4\pi q^2\sigma_+ d/\varepsilon_i & \text{for } \pi d^2\sigma_+\ll 1 \\ 4q^2\sigma_+ r_F E(r/r_F)/\varepsilon^* & \text{for } \pi d^2\sigma_+\gg 1 \end{cases}. \tag{10}$$

Here, $E(r/r_F)$ is a complete elliptic integral of the second kind and $\varepsilon^*=(\varepsilon_i+\varepsilon_s)/2$.

We shall consider the case when the thickness of the insulator is much less than the thickness of the Schottky layer ($d\ll L$). Then, the expression (3) for $v(r)$ can be represented approximately in the form

$$v(r)=-\frac{q^2}{\varepsilon^*}\left[\frac{1}{r}-\frac{1}{(r^2+(2d)^2)^{1/2}}\right]. \tag{11}$$

The energy position of a vacant donor E_+ can be found by averaging the potential of all the remaining charges over their positions bearing in mind that the charged donors can occur only outside a circle of radius r_F centered at the point of location of the vacant donor. This gives

$$E_+=-E_0+V_s+V_c(r=0,\ r_F), \tag{12}$$

and hence we find that vacant donors have the same energy and are located at Δ above the Fermi level, where

$$\Delta=E_+-E(r_F)=V_c(r=0,\ r_F)-V_c(r_F,\ r_F)-v(r_F). \tag{13}$$

We can thus see that there is a gap between the vacant and filled levels in the spectrum of the surface states and the density of the vacant donors is delta-like. The gap obtained is in fact associated with allowance for the correlation in the distribution of the charged centers.

We shall now find the relationship between the charged donor concentration σ_+ and the Fermi radius r_F. We shall assume that the donors in the plane of the SI interface obey the Poisson distribution, i.e., that the probability of finding m donors in a circle of radius r is given by

$$P_m(r)=\frac{(\pi r^2\sigma)^m}{m!}\exp(-\pi r^2\sigma). \tag{14}$$

We shall divide the surface into circle of radii r_F. The probability that a given circle r_F contains m donors is given by Eq. (14). By definition of r_F, out of the m donors in a circle of radius r_F, only one is charged and the other $m-1$ are neutral. Then, the average neutral donor concentration σ_0, equal to $\sigma-\sigma_+$, can be found from

$$\sigma_0=\frac{1}{\pi r_F^2}\sum_{m=1}^{\infty}(m-1)P_m(r_F),$$

and hence we obtain

$$\sigma_+=\frac{1}{\pi r_F^2}(1-\exp(-\pi r_F^2\sigma)). \tag{15}$$

In fact, Eq. (15) shows that in a circle of radius r_F there can be only one charge donor on condition that this circle contains at least one donor.

We shall find the dependence of the surface-state occupancy on the depending of the semiconductor bands. The system (8), (15) defines implicitly the self-consistent dependence $\sigma_+(V_s)$. We shall rewrite Eq. (8) subject to Eqs. (7) and (9) in the following form

$$V_c(r_F,\ r_F)+v(r_F)=E_F, \tag{16}$$

where E_F represents the separation of the unperturbed donor level from the Fermi level:

$$E_F=\mu+E_0-V_s. \tag{17}$$

We shall solve the system (15), (16) by expressing r_F in terms of σ_+. This is easily done in the case of low and high concentrations of the charged donors. It follows from Eq. (15) that

$$r_F=\begin{cases} (\pi\sigma_+)^{-1/2}(1-{}^1/_2\exp(-\sigma/\sigma_+)) & \text{for } \sigma_+\ll\sigma \\ (\pi\sigma)^{-1/2}[2(1-\sigma_+/\sigma)]^{1/2} & \text{for } \sigma-\sigma_+\ll\sigma \end{cases}. \tag{18}$$

Substituting $r_F(\sigma_+)$ from Eq. (18) into Eq. (16), we obtain the explicit relationship between E_F and σ_+:

$$\begin{aligned} E_F&=\frac{4\pi q^2\sigma_+ d}{\varepsilon_i}\left(1-\frac{1}{2}\frac{\varepsilon_i}{\varepsilon^*}(\pi\sigma_+)^{1/2}d\right) && \text{for } \pi d^2\sigma_+\ll 1,\ \sigma_+\ll\sigma; \\ E_F&=\left(\frac{4}{\pi}-1\right)\frac{q^2}{\varepsilon^*}(\pi\sigma_+)^{1/2} && \text{for } \pi d^2\sigma_+\gg 1,\ \sigma_+\ll\sigma; \\ E_F&=-\frac{q^2}{\varepsilon^*}(\pi\sigma)^{1/2}\left[2\left(1-\frac{\sigma_+}{\sigma}\right)\right]^{-1/2} && \text{for } \pi d^2\sigma_+\gg 1,\ \sigma-\sigma_+\ll\sigma. \end{aligned} \tag{19}$$

The general form of the function $\sigma_+(E_F)$, described by Eqs. (15) and (16), is shown in Fig. 2 (curve 1). For comparison, this figure includes the dependence $\sigma_+(E_F)$ for a monoenergetic level without allowance for

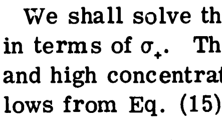

FIG. 2. Dependences of δ_+ on the Fermi level position in the case of a monoenergetic donor center on the surface: 1) calculated allowing for the Coulomb interaction between the centers; 2) calculated ignoring the Coulomb interaction.

the Coulomb interaction (line 2). We can see from Fig. 2 that the dependence $\sigma_+(E_F)$ is multivalued in respect of E_F and, consequently, in respect of V_s. We shall now demonstrate the consequences of this dependence.

4. SMALL-SCALE DENSITY OF STATES

We shall calculate the density of states $N_{ss}(E)$ for a fixed bending of the semiconductor bands V_s and a corresponding fixed value of E_F. We shall find the density of states below the Fermi level. We shall do this by calculating the concentration of neutral donors $N(r)$ which are located at distances smaller than r $(r \leq r_F)$ from the nearest charged donor.

We shall divide the SI interface into circles of radii r_F. By definition of r_F, each of these circles contains one charged donor if the circle does contain at least one donor. We shall consider circles containing m donors. The probability of finding such circles is given by Eq. (14) and is $P_m(r_F)$. Each of these circles can be divided into circles of radius r smaller than r_F. The probability that out of m donors located in a circle of radius r_F there are n donors $(n \leq m)$ in a circle of radius r is

$$C_m{}^n (r^2/r_F{}^2)^n (1-r^2/r_F{}^2)^{m-n}. \qquad (20)$$

The probability that among these n donors there is a charged one is equal to the ratio n/m. The product of these probabilities governs the probability that $n-1$ donors are located at distances smaller than r from the charged donor:

$$P_m(r_F)\frac{n}{m}C_m{}^n\left(\frac{r^2}{r_F{}^2}\right)^n\left(1-\frac{r^2}{r_F{}^2}\right)^{m-n}. \qquad (21)$$

In order to determine the concentration of neutral donors, we have to sum the probability (21) with a weighting factor $n-1$ over n and m, and multiply the result by the density of small circles $1/\pi r^2$. This gives

$$N(r)=\frac{1}{\pi r^2}\sum_{m=2}P_m(r_F)\sum_{n=2}\frac{(n-1)n}{m}C_m{}^n\left(\frac{r^2}{r^2}\right)^n\left(1-\frac{r^2}{r^2}\right)^{m-n}. \qquad (22)$$

Summation over n and m and application of Eq. (15) shows that

$$N(r)=(\sigma-\sigma_+)r^2/r_F{}^2. \qquad (23)$$

The density of neutral states is given by

$$N_{ss}(E)=\frac{\partial N(r)}{\partial r}\frac{\partial r}{\partial E}\bigg|_{E(r)=E}. \qquad (24)$$

Using Eqs. (7), (11), and (23), we find from Eq. (24) that in the case of low concentrations of charged donors $(\pi d^2\sigma_+ \ll 1)$ this density is

$$N_{ss}(E)=\begin{cases}\dfrac{2(\sigma-\sigma_+)}{3|v(r_F)|}\left[1-\dfrac{\mu-E}{v(r_F)}\right]^{-5/3} & \text{for } r\gg d\\[2ex] \dfrac{2(\sigma-\sigma_+)}{|v(r_F)|}\left[1-\dfrac{\mu-E}{v(r_F)}\right]^{-3} & \text{for } r\ll d\end{cases}. \qquad (25)$$

In the case of high concentrations of charged donors $(\pi d^2\sigma_+ \gg 1)$ the density of the states below the Fermi level is

$$N_{ss}(E)=\frac{2(\sigma-\sigma_+)}{|v(r_F)|}\left[1-\frac{\mu-E}{v(r_F)}\right]^{-3}. \qquad (26)$$

It follows that the approximation of the potential of the nearest charged centers predicts a monotonic fall of the density of neutral donor states below the Fermi level, whereas vacant donors have the same energy and are separated from the neutral donors by a gap Δ.

The energy distribution of the vacant states is due to fluctuations of the distances between the charged centers. This has to be allowed for when the fluctuation potential is considered in the approximation of two charged centers. The potential of charged centers can be determined by drawing a circle of radius R around a pair of the nearest charged donors located symmetrically. The radius of this circle is found from the requirement of electrical neutrality of the system: $R=(2/\pi\sigma_+)^{1/2}$. The potential due to the charge inside the circle is allowed for exactly and the potentials of all the other charges outside the circle R are averaged over their positions.

We shall consider the case $\pi d^2\sigma_+ \gg 1$. According to Eq. (11), this inequality allows us to write down the energy of the charged donors $E_+(r)$ separated by a distance r and we can do this in a unified form which applies to low and high concentrations σ_+ $(\sigma_+ \ll \sigma$ and $\sigma-\sigma_+ \ll \sigma)$:

$$E_+(r)=-E_0+V_s+\frac{4q^2\sigma_+R}{\varepsilon^*}E\left(\frac{r}{2R}\right)-\frac{q^2}{\varepsilon^* r}. \qquad (27)$$

Here, $E(r/2R)$ is a complete elliptic integral of the second kind. The third term in Eq. (27) gives the potential at a distance $r/2$ from the center of a negatively charged disk of radius R with a homogeneous charge density $-q\sigma_+$. The last term in Eq. (27) represents the Coulomb interaction between two charged donors separated by a distance r.

The expression (27) has a maximum at a point r_0 $(r_0 < R)$. Thus, $E_+(r_0)$ is the maximum energy of charged donors in the two-center approximation (Fig 3).

We shall find r_0 and $E_+(r_0)$ by introducing a variable $x=(r/2R)^2$, when the equation describing the maximum of $dE_+(r)/dr=0$ reduces to

$$E'(x)+\pi x^{-3/2}/32=0.$$

A numerical solution of this equation gives $x=x_0 = \sin^2 36.68°$. Consequently, we obtain

$$r_0=0.953\sigma_+{}^{-1/2}, \qquad (28)$$

$$E_+(r_0)=-E_0+V_s+V_c. \qquad (29)$$

In the two-center approximation the value of V_c differs

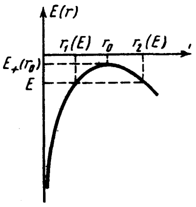

FIG. 3. Potential of charged donors plotted as a function of the distance between donors in the two-center approximation.

slightly from the value $V_c(r=0, r_F)$ obtained earlier in the one center approximation [see Eq. (10)] and it is

$$V_c = 1{,}96\frac{q^2}{\varepsilon^*}(\pi\sigma_+)^{1/2}. \qquad (30)$$

It follows from the nature of the potential (27) that from the energy point of view of the two charged centers are most likely to be separated by a distance r_0 and have the energy $E_+(r_0)$. A vacant donor may have an energy E smaller than $E_+(r_0)$ if in a ring bounded by circles of radii r_1 and $r_2(r_1<r_2)$ there is not even one donor. Here, r_1 and r_2 are given by the equation $E_+(r)=E$ (Fig. 3). Thus, the concentration of charged donors with energies in the interval from E to $E+dE$ is given by the product of the probability of the appearance of a donor at a distance from r_1 to r_1+dr_1 and from r_2 to r_2+dr_2, multiplied by the probability of the absence of a donor in a ring of radii r_1 and r_2.

Consequently, the following expression is obtained for the density of states of charged donors

$$N_{ss}(E)=\frac{4\sigma}{R^2}\left[r_2(E)\left|\frac{dr_2(E)}{dE}\right|+r_1(E)\left|\frac{dr_1(E)}{dE}\right|\right]\exp\{-\pi[r_2^2-r_1^2]\sigma\}, \qquad (31)$$

which can be conveniently transformed to

$$N_{ss}(E)=\sigma_+\frac{d}{dE}\{\exp(-\pi[r_2^2(E)-r_1^2(E)]\sigma)\}. \qquad (32)$$

The explicit dependences of r_2 and r_1 on E can be obtained by expanding $E_+(r)$ near its maximum value reached at the point r_0:

$$E_+(r)=E_+(r_0)+{}^1/_2E''(r_0)(r-r_0)^2. \qquad (33)$$

Calculations give the following density of states of charged donors

$$N_{ss}(E)=\frac{\sigma\alpha}{2V_c}\left[\frac{V_c}{E_+(r_0)-E}\right]^{1/2}\exp\left\{-\alpha\frac{\sigma}{\sigma_+}\left(\frac{E_+(r_0)-E}{V_c}\right)^{1/2}\right\}, \qquad (34)$$

where

$$\alpha=32\left[2x_0(1-x_0)\frac{E(x_0)-\pi/16x_0^{1/2}}{E(x_0)+\pi(1-x_0)/16x_0^{1/2}}\right]^{1/2}\approx 17.$$

We can see from Eq. (34) that in the case of small $\sigma_+(\sigma_+\ll\sigma)$ the dispersion of the potential of vacant donors is small compared with the gap between the vacant and filled donors. Hence, charged donors are located at practically the same distances close to r_0 and the gap between the vacant and occupied donors is filled to a degree which is exponentially small (Fig. 4a).

In the range of high values of $\sigma_+(\sigma-\sigma_+\ll\sigma)$ the smearing of the density of states of vacant donors increases in accordance with Eq. (34) and r_F then becomes much smaller than r_0 [see Eq. (18)]. Then, the expression for $E_+(r)$ when $r\ll r_0$ can be represented approximately in the form

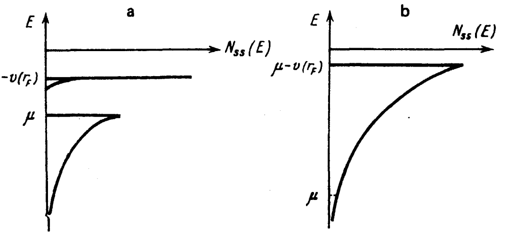

FIG. 4. Surface state density: a) low concentration of charged donors ($\sigma_+\ll\sigma$); b) high concentration of charged centers ($\sigma-\sigma_+\ll\sigma$).

$$E_+(r)=-E_0+V_s+V_c-q^2/\varepsilon^*r. \qquad (35)$$

Using Eqs. (32) and (35), we find that in the range of high σ_+ the expression for the density of charged states near the Fermi level is

$$N_{ss}(E)=\frac{2(\sigma-\sigma_+)}{|v(r_F)|}\left[1-\frac{\mu-E}{v(r_F)}\right]^{-3}\exp\left(-\frac{2\sigma}{\sigma_+}\right). \qquad (36)$$

Thus, in the range of high σ_+ the characteristic energy of the density smearing is, according to Eq. (36), $|v(r_F)|$, i.e., it is of the order of the gap so that the gap between the vacant and filled states disappears (Fig. 4b).

5. LARGE-SCALE FLUCTUATIONS OF THE POTENTIAL

In the preceding section we have allowed for the existence of a small-scale inhomogeneous potential associated with the discrete nature of the charges and with the fluctuations of the distance between the nearest charges. We shall now find a large-scale fluctuation potential which is due to fluctuations of the charge density $\Delta\sigma_+$ over distances much greater than the average separation between charged centers.

Fluctuations of the large-scale potential $\tilde{V}$ with a certain scaling length R depend on fluctuations of the charge concentration on the surface $\Delta\sigma_+$ and these fluctuations are a function of deviation of the total donor concentrations from the average value $\Delta\sigma$ and, moreover, of the potential $\tilde{V}$ itself. Therefore, the problem of the large-scale fluctuation potential should be solved in a self-consistent manner.

The relationship between the large-scale fluctuation potential and $\Delta\sigma$ can be found by solving the Poisson equation in the fluctuation range together with the equations of states (15) and (16) obtained by considering small-scale fluctuations and describing the relationship between $\Delta\sigma_+$, $\Delta\sigma$, and $\tilde{V}$.

The solution of the Poisson equation for $\tilde{V}$ inside a fluctuation obtained on the assumption of a homogeneous distribution of the surface charge in the fluctuation region is

$$\tilde{V}(r)=\begin{cases}-4\pi q^2\Delta\sigma_+d/\varepsilon_1 & \text{for } R\gg d\\ -4q^2\Delta\sigma_+RE(r/R)/\varepsilon^* & \text{for } R\ll d\end{cases}. \qquad (37)$$

Since $E(r/R)$ is a smooth function varying from $\pi/2$ to 1 as r/R varies from 0 to 1, we shall solve simultaneously Eqs. (15), (16), and (37) ignoring the coordinate dependence of the potential in the fluctuation region and we shall assume that the potential of this region is equal to the potential at the center af the fluctuation.

The equation defining the local Fermi radius in a large-scale fluctuation with a deviation of the potential from the average $\tilde{V}$ is

$$E(r_F)=-E_0+V_c+v(r_F)+V_s+\tilde{V}=\mu. \qquad (38)$$

The system of equations (15), (37), and (38) defines the dependences of $\Delta\sigma_+$ and $\tilde{V}$ on $\Delta\sigma$. These dependences can be obtained explicitly in the two limiting cases: $\sigma_+ \ll \sigma$ and $\sigma - \sigma_+ \ll \sigma$.

If the concentration of charged donors is low ($\pi d^2\sigma_+ \ll 1$), we obtain the following relationships from the above equations:

$$\Delta\sigma_+ = \Delta\sigma \exp\left(-\frac{\sigma}{\sigma_+}\right), \quad \tilde{V} = -\frac{4\pi q^2 d}{\varepsilon_1}\Delta\sigma \exp\left(-\frac{\sigma}{\sigma_+}\right). \tag{39}$$

The Poisson distribution of donors for large fluctuation radii ($\pi R^2\sigma \gg 1$) reduces to the Gaussian distribution for $\Delta\sigma$, which can be used to calculate readily the dispersion of the large-scale potential $\gamma + (\overline{\tilde{V}^2})^{1/2}$:

$$\gamma = \frac{4q^2 d}{\varepsilon_1 R}(\pi\sigma)^{1/2} \exp\left(-\frac{\sigma}{\sigma_+}\right). \tag{40}$$

It follows from this expression that in the case of low concentrations of charged donors the dispersion of the large-scale fluctuation potential is exponentially small. It follows that in the case of small values of σ_+ the small-scale density is practically unsmeared by the large-scale fluctuation potential. In particular, the gap between the vacant and filled states is still retained.

If the donor concentration is high, $\sigma - \sigma_+ \ll \sigma$, similar calculations show that

$$\Delta\sigma_+ = \Delta\sigma, \quad \tilde{V} = -\frac{2\pi q^2}{\varepsilon^*} R\Delta\sigma, \quad \gamma = 2\frac{q^2}{\varepsilon^*}(\pi\sigma)^{1/2}. \tag{41}$$

It is clear from these expressions that in the case of high σ_+ the dispersion due to the large-scale potential is much less than the dispersion of the small-scale potential which, according to Eq. (36), is $|v(r_F)|$.

We can thus say that for any relationship between σ_+ and σ, we can ignore the large scale fluctuation potential compared with the small-scale potential.

6. WIGNER CRYSTALLIZATION AND ELEMENTARY EXCITATIONS

We shall consider the problem of the Wigner crystallization of charged donors at the SI interface. We have shown that in the case of low concentrations of charged donors ($\sigma_+ \ll \sigma$) the magnitudes of the small- and large-scale fluctuation potentials acting on vacant donors are exponentially small compared with the Coulomb interaction between the nearest charged centers [see Eqs. (34) and (40)]. This means that the distance between charged donors hardly fluctuates in the range of low values of σ_+. This is to be expected on physical grounds because the number of possible locations of a charged donor increases on reduction in σ_+. Then, the Coulomb repulsion ensures that charged donors are located at places favored by the energy considerations, forming a crystal structure at the SI interface (Wigner crystal).

In the case of a periodic distribution of charged donors we can readily calculate the gap between the vacant and filled states; this can be done on a computer specifying the type of the lattice of charged donors. In particular, for a triangular grating allowing for the interaction with 1.6×10^5 nearest charged donors, we find that the gap Δ is

$$\Delta = 0{,}95\frac{q^2}{\varepsilon^*}(\pi\sigma_+)^{1/2}. \tag{42}$$

This gap agrees with the value obtained by us earlier [see Eq. (13)]. It follows that the approximation of the nearest charged center describes well the potential. The corrections to the potential appear because of fluctuations in the positions of charged donors. Returning to the results of a calculation of the density of states of vacant donors (34) and of the dispersion of the large-scale potential (40), we find that the small parameter occurring in the corrections to the potential which allows for the interaction only with the nearest charged center is $\exp(-\sigma/\sigma_+)$. This parameter is much smaller than unity in the range of low concentrations σ_+. However, even in the case of high concentrations σ_+, the approximation of the nearest charged center is valid in the case of high energies (near the Fermi level). At these energies the distance between donors should be of the order of r_F. Then, the deviation from the potential obtained in the approximation of the nearest charged center occurs if there is an additional charged donor at a distance of the order of r_F. The ratio of the probabilities of finding three or two donors in a circle of radius r_F represents that correction to the density near the Fermi level which appears as a result of allowance for the presence of two charged donors. This ratio is $\pi r_F^2\sigma \approx 1 - \sigma_+/\sigma$.

A somewhat more "stringent" parameter $(1 - \sigma_+/\sigma)^{1/2}$ appears in the range of high concentrations σ_+ if we compare the small-scale potential at the Fermi level $v(r_F)$ and the dispersion of the large-scale potential (41). Thus, throughout the range of variation of σ_+ we can derive a small parameter p which can be used in the calculation of the potential in the approximation of the nearest charged center:

$$p = (1 - \sigma_+/\sigma)^{1/2}\exp(-\sigma/\sigma_+). \tag{43}$$

It should be pointed out that the energy gap between the vacant and filled states is essentially a Coulomb gap.[9-12] The "rigidity" of this gap in the range of small values of σ_+ is due to the fact that we have considered monoenergetic donor centers. The appearance of a rigid gap in this situation was pointed out by Baranovskiĭ *et al.*[12] In the range of high values of σ_+ the absence of correlation in the donor distribution destroys the gap. The density-of-states gap can be observed only by tunnel spectroscopy methods.[13] The gap between the vacant and filled centers gives rise to an additional voltage drop when electrons tunnel away from the surface and back to the surface.

We shall now consider the problem of elementary excitations under the Wigner crystallization conditions ($\sigma_+ \ll \sigma$). According to the classification in Ref. 12, we have to distinguish dipole and charged excitations associated with an electron transition from a filled state to a vacant center (pair excitations). By definition, an excitation with a jump of length $r < r_0$ is of the dipole type, whereas an excitation with $r > r_0$ is charged. Here, r_0 denotes a characteristic length equal to $q^2\varepsilon\Delta$ (Δ is the width of the Coulomb gap). According to Eq. (13), in the case of the system considered here the length in question is identical with the Fermi radius, i.e., with the Wigner cell size, thus transitions within a cell are of the dipole type, whereas transitions between cells are charged.

We shall now calculate the energy of elementary excitations. We shall assume that there is a Wigner lattice and the lattice site coordinates are r_n. The random distribution of donors on the surface causes real positions of the charged donors to fluctuate weakly relative to the lattice sites. A deviation of the position of a charged donor from the lattice site within the n-th cell will be denoted by r_{1n}. The energy position of such a charged donor is given by

$$E_+(r_{1n})=-E_0+V_s+V_c(r_{1n},\ r_F), \tag{44}$$

where $V_c(r_{1n}, r_F)$ is given by Eq. (10). The energy of a neutral donor located in the m-th cell at a point r_{2m} is

$$E_0(r_{2m})=-E_0+V_s+V_c(r_{2m},\ r_F)+v(r_{1m}-r_{2m}), \tag{45}$$

where r_{1m} is the position of a charged donor in this cell. The work ω needed to transfer an electron from a filled site at $\mathbf{r}_{2m}$ to an empty site at $\mathbf{r}_{1n}$ is

$$\omega=V_c(r_{1n},\ r_F)-V_c(r_{2m},\ r_F)-v(\mathbf{r}_{1m}-\mathbf{r}_{2m})+v(\mathbf{r}_{1m}-\mathbf{r}_{2n}+\mathbf{r}_{mn}), \tag{46}$$

where $\mathbf{r}_{mn}=\mathbf{r}_m-\mathbf{r}_n$. Hence, we can see that the energies of dipole and charged excitations are given by expressions which have different structures. In the case of dipole excitations the values of m and n are equal and the last two terms in Eq. (46) balance out. Consequently the energy of a dipole excitation is given by

$$\omega=V_c(r_{1n},\ r_F)-V_c(r_{2n},\ r_F). \tag{47}$$

The maximum energy of dipole excitations ω_m is identical with the minimum energy of charged excitations and

$$\omega_m=\Delta+v(r_F)=V_c(r=0,\ r_F)-V_c(r_F,\ r_F).$$

It follows from Eq. (47) that the presence of a gap in the density of states does not give rise to a gap in the energy of elementary excitations, since in the limit $r_{2n}\to r_{1n}$ we have $\omega\to 0$.

In the case of transitions between cells an increase in the distance between the cells causes the minimum excitation energy to approach Δ. Thus, the Coulomb gap appears only for transitions of large distances. In fact, it follows from Eq. (46) that transitions of energy lower than Δ occur in a bounded part of space, which is in agreement with the principle of compactness discussed in Ref. 12.

We shall find the density of states of excitations $\Phi(\omega)$. According to Ref. 12, we can do this by calculating the probability that in an interval dr_{1n} there is a charged donor, whereas in the interval dr_{2n} there is an empty donor, and the energy required for this transition is ω. This probability is

$$2\pi r_{1n}\sigma\exp(-\pi r_{1n}^2\sigma)\,dr_{1n}\cdot 2\pi r_{2n}\sigma\,dr_{2n}\cdot\delta(V_c(r_{1n},\ r_F)-V_c(r_{2n},\ r_F)-\omega).$$

Multiplying this probability by the number of cells (σ_+) and integrating with respect to r_{1n} and r_{2n}, we obtain the required density of states of excitations:

$$\Phi(\omega)=2\sigma/|v(r_F)|. \tag{48}$$

It should be noted that this density of states of excitations is identical with the density of states at the Fermi level given by Eq. (26). It is clear from Eq. (48) that the density of excitations remains constant in the range of small values of ω. It is then easily demonstrated that the low-temperature specific heat is proportional to temperature. We shall now make some comments on the low-temperature hopping conduction under the Wigner crystallization conditions. Naturally such long-range conduction may occur because of excitations. However, this process is unlikely because the minimum activation energy is of the order of Δ and the overlap of the wave functions is exponentially small. It is more probable that charge is transferred because of electron transitions from the nearest filled to a vacant donor, and such dipole excitations create a potential gradient in neighboring cells which facilitates activation-free transitions of electrons in these cells. We can thus say that the low-temperature hopping conduction is due to dipole excitations undergoing a relay type of transport: a transition within one cell facilitates electron transitions in neighboring cells, i.e., motion of the crystal as a whole is expected.

The average activation energy $\bar{\omega}$ for this mechanism can be determined by assuming that transitions occur on the average over distances $\sim(\pi\sigma)^{-1/2}$:

$$\bar{\omega}\approx\Delta(\sigma_+/\sigma).$$

The applications of an electric field reduces the activation energy of conduction:

$$\bar{\omega}\approx\Delta(\sigma_+/\sigma)-qF/\sigma^{1/2}.$$

It follows from this relationship that in electric fields $F\geqslant\Delta\sigma_+/q\sigma^{1/2}$ we can expect activation-free hopping conduction.[11]

7. DEPENDENCE OF THE CAPACITANCE OF AN MIS STRUCTURE ON THE EXTERNAL VOLTAGE

We shall consider the effects resulting from the dependence $\sigma_+(E_F)$ (Fig. 2). We shall do this by calculating the change in the total capacitance C of an MIS structure on the external voltage V_g. The low-frequency capacitance of an MIS structure measured using a small alternating signal is given by

$$C(V_g)=dq\sigma_m/dV_g. \tag{49}$$

We shall find this dependence by writing down the system of equations describing the distribution of the external voltage between the insulator and the semicon-

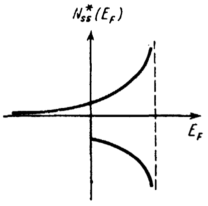

FIG. 5. Effective density of surface states.

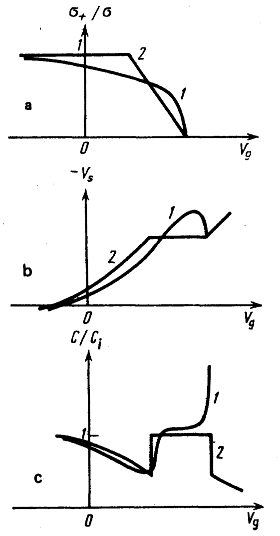

FIG. 6. Dependences $\sigma_+(V_g)$, $V_s(V_g)$, and $C(V_g)$ for the case monoenergetic donor centers on the surface and subject to allowance for the Coulomb interaction between such centers (curve 1) and without allowance for the interaction (curve 2).

ductor, and the continuity of electrostatic induction at the interface:

$$V_g=F_i d-V_s/q, \tag{50}$$

$$4\pi q\sigma_m=\varepsilon_i F_i=\varepsilon_s F_{ss}-4\pi q\sigma_+, \tag{51}$$

where F_i and F_{ss} are the average electric fields in the insulator and semiconductor measured at the SI interface. The electric field on the semiconductor surface with a depletion Schottky layer can be expressed in terms of the surface potential

$$F_{ss}=(-8\pi N_a V_s/\varepsilon_s)^{1/2}. \tag{52}$$

Equations (50)–(52) supplemented by the dependence $\sigma_+(V_s)$ from Eqs. (15) and (16) give the dependence of the capacitance of an MIS structure on the external voltage. Differentiating Eq. (51) with respect to V_g, we find that subject to Eq. (52) the capacitance is given by

$$C=-C_s\frac{dV_s}{d(qV_g)}-\frac{dq\sigma_+}{dV_g},\quad C_s=\frac{\varepsilon_s}{4\pi L}. \tag{53}$$

Equation (50) together with Eqs. (51) and (52) can be transformed to

$$V_g=-\frac{q\sigma_+}{C_i}-\frac{V_s}{q}+\frac{d}{\varepsilon_i}(-8\pi N_a\varepsilon_s V_s)^{1/2},\quad C_i=\frac{\varepsilon_i}{4\pi d}. \tag{54}$$

Differentiating the above expressions with respect to V_s and σ_+, we find

$$\frac{dV_s}{d(qV_g)}=-\frac{\varepsilon_i}{\varepsilon_i}\left[1-\frac{4\pi q^2 d}{\varepsilon_i}\frac{d\sigma_+}{dE_F}\right]^{-1}, \tag{55}$$

$$\frac{d(q\sigma_+)}{dV_g}=-C_i\left[1-\frac{\varepsilon_i}{4\pi q^2 d}\frac{dE_F}{d\sigma_+}\right]^{-1}. \tag{56}$$

The right-hand sides of these relationships include a quantity $d\sigma_+/dE_F$ which, like $C(V_g)$, is an observable quantity representing the effective density of states at the SI interface N^*_{ss} (Ref. 14):

$$N_{ss}^*=d\sigma_+/dV_s=-d\sigma_+/dE_F. \tag{57}$$

Using Eqs. (8) and (17) or the approximate expression (21), we can obtain $N^*_{ss}(E_F)$. This dependence is shown qualitatively in Fig. 5. The dependence is multivalued in respect of E_F, i.e., with respect to V_s, but is single valued with respect to V_g.

Substituting $N^*_{ss}(E_F)$ in Eq. (53) subject to allowance for Eqs. (55) and (56), we obtain the capacitance of an MIS structure which is conveniently expressed in terms of σ_+:

$$\begin{aligned}
&C=\frac{4\varepsilon^*\varepsilon_i C_i}{3\varepsilon_i^2(\pi\sigma_+)^{1/2}d}\quad \text{for}\ \pi d^2\sigma_+\ll 1,\ \sigma_+\ll\sigma;\\
&C=C_i\left(1+\frac{\varepsilon_i}{8\varepsilon^*(\pi\sigma_+)^{1/2}d}\right)\quad \text{for}\ \pi d^2\sigma_+\gg 1,\ \sigma_+\ll\sigma;\\
&C=\left(\frac{1}{C_s}+\frac{1}{C_i}\right)^{-1}-\frac{2\varepsilon^*\varepsilon_i}{\pi\sigma\varepsilon_i^2}[2\pi(\sigma-\sigma_+)^3]^{1/2}\quad \text{for}\ \pi d^2\sigma_+\gg 1,\ \sigma-\sigma_+\ll\sigma.
\end{aligned} \tag{58}$$

The qualitative form of the dependences $\sigma_+(V_g)$, $V_s(V_g)$, and $C(V_G)$, obtained above is shown in Fig. 6. At low values of σ_+ the capacitance of an MIS structure becomes greater than C_i and, in the limit $\sigma_+\to 0$, we have $C\to\infty$ (Fig. 6c).

The main features of the above model approach most closely the experimental results of Harstein and Fowler,[15] who investigated an MIS structure based on silicon and with sodium ions (monoenergetic donor centers) on the semiconductor surface. They observed a nonmonotonic dependence of the conductivity along the surface of a semiconductor as a function of V_g, which can be matched to our nonmonotonic dependence $V_s(V_g)$.

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[1)] We have derived this inequality using the fact that the main contribution to the dispersion of the fluctuation potential is made by small-scale fluctuations so that an estimated value of ΔL is the change in the Schottky layer thickness on appearance of a unit point charge on the semiconductor surface.

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