Surface recombination and fluctuation surface states

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A new tunnel-thermogeneration mechanism is proposed for the realization of generation and recombination of carrier on a semiconductor-insulator interface. The mechanism comprises a combined process that includes ordinary capture (generation) of carriers in electron and hole fluctuation potential wells located on the interface at a certain distance from one another, and subsequent tunneling of the carriers between wells of opposite type. The methods of the theory of optimal fluctuations are used to calculate the dependence of the effective rate of surface recombination on the average surface potential. It is shown that at relatively high temperatures the rate of the recombination process limits the tunneling, and at relatively low temperatures the limit is imposed by thermogeneration. A simple qualitative criterion is obtained for distinguishing between the proposed mechanism and the traditional model of recombination via a monoenergetic surface state.

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In Ref. 1 it was proposed to describe the dielectric properties of a semiconductor-insulator interface by the so-called fluctuation model of surface states. It presupposes the presence, on the interface, of randomly distributed charged centers that produce a three-dimensional fluctuation relief of the electrostatic potential in the subsurface layer of the semiconductor. This random relief is described by a correlation function

$$K(z,z'\ R)\approx 2\Delta^2 \ln\left(\frac{4R_c}{z+z'+[(z+z')^2+R^2]^{1/2}}+1\right), \quad (1)$$

where $\Delta = e^2(\pi\sigma)^{1/2}/x$ is the characteristic energy of the fluctuations, $\sigma \equiv \sigma^+ + \sigma^-$ is the summary average surface density of the positively and negatively charged centers on the interface, $x = \frac{1}{2}(\varepsilon_i + \varepsilon_s)$ is the effective dielectric constant (ε_i and ε_s are the dielectric constants of the insulator and of the semiconductor), z and R are the normal and tangential coordinates ($z = 0$ corresponds to the interface), and $R_c = (\sigma/\pi)^{1/2}(Q_n + Q_p)^{-1}$ is the radius of the nonlinear electron-hole screening (Q_n and Q_p are the surface densities of the bound electron and hole charges).

At thermodynamic equilibrium the electrons and holes fill states localized at the interface at the fluctuation-relief minima and maxima, whose energies lie below (above) the Fermi level. The corresponding density of states is determined mainly by the probability of realizing fluctuation potential wells of the required depth, and constitutes a superposition of exponential electron and hole "tails." It was found that the hyperbolic expression obtained in Ref. 1 for the effective energy density of such states

$$N_{ss}(\varepsilon)=\frac{1}{\Delta}\frac{(\sigma/\pi)^{5/8}}{(4a_n a_p)^{3/8}}\exp\left(-\frac{E_g}{4\Delta}\right)\mathrm{ch}\left(\frac{\varepsilon-\varepsilon_0}{2\Delta}\right), \quad \varepsilon_0\approx\frac{E_g}{2}, \quad (2)$$

where a_n and a_p are the Bohr radii of the electron and hole while E_g is the width of the forbidden band, agrees well with the experimentally observed surface-state spectra.[2] The latter determine, by analyzing the change of the charge captured at the interface with change of the surface potential[1)] φ. Then

$$\varepsilon=\varphi+\mu=\varphi+T\ln(N_v/p_0),$$

where p_0 is the hole density in the substrate and N_v is the state density in the valence band.

It is known that besides capturing carriers the semiconductor-insulator interface exhibits also a definite generation-recombination activity. The rate of surface recombination that characterizes this activity also depends strongly on the surface potential. Usually this dependence is interpreted by using the simplest theoretical model of recombination via a monoenergetic surface state whose energy is close to the midpoint of the forbidden band. This model, which is analogous to the Shockley-Read theory for recombination in the bulk, leads to the bell-shaped relation

$$S(\varphi)=N_t(\gamma_n\gamma_p)^{1/2}\frac{n_0+p_0}{2n_i}\left[\mathrm{ch}\frac{(\varphi-\varphi_B-\alpha)}{T}+\mathrm{ch}\frac{\varepsilon_t-\alpha}{T}\right]^{-1}, \quad (3)$$

which approximates quite well the experimental results. Here N_t is the surface density of these hypothetical recombination centers, ε_t is their energy reckoned from the middle of the forbidden band, γ_n and γ_p are coefficients of the electron and hole capture, respectively,

$$\alpha=\tfrac{1}{2}T\ln(\gamma_p/\gamma_n); \qquad n_i=(N_cN_v)^{1/2}\exp(-E_g/2T)$$

is the intrinsic carrier density (N_c is the density of states in the conduction band), and φ_B is the surface potential at which the densities of the majority and minority carriers are equal on the interface ($n = p = n_i$). We have referred to these recombination surface states as hypothetical, since a comparison of the experimental $S(\varphi)$ dependences with Eq. (3) yields neither their densities nor their capture coefficients.

There are definite indications of at least a qualitative connection between surface recombination and the capture surface states whose energy spectrum is quasi-continuous. It was noted already in Refs. 3 and 4 that in structures with high density of surface states are observed high surface-recombination states, just as different thermochemical actions

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on the interface cause the capture density of states and the rate of the surface recombination to change "in one direction." In the present paper, as a further development of the concepts of fluctuation surface states,[1] we investigate a generation-recombination process in the subsurface layer of a semiconductor with a fluctuation surface relief (1). As a result we shall obtain the dependences of the effective surface-recombination rate on the average surface potential; these dependences are close to the bell-shaped $S(\varphi)$ curves both in shape and in magnitude. We note in particular that in the Conclusion we shall formulate a clear qualitative criterion by which to distinguish the proposed recombination process from the traditional mechanism of recombination via a monoenergetic surface level.

It is perfectly clear that when analyzing the generation-recombination "capabilities" of the fluctuation relief (1) we must take into consideration the tunneling of an electron from a subsurface electron potential well into a hole well located somewhere in the neighborhood of a hole well of corresponding depth, since the electron and hole localized states, whose superposition yields the spectrum (2), are single-band. It is natural to expect in this case the principal role to be played by rather deep states (with binding energy on the order of the half-width of the forbidden band) and, as is usual in similar cases,[5] we shall take into account only the ground state in such fluctuation wells (single-particle filling of the fluctuations).

The elementary act of the proposed recombination mechanism consists of three stages: 1) capture a free electron whose energy lies higher than the average position of the conduction-band edge on the interface—the percolation level—by a bound electron state with energy $-\delta\varphi+\hbar^2/2m_nz_0^2$ in an electron potential well having a depth $\delta\varphi$ and a characteristic dimension[2] z_0; 2) capture of a free hole by a bound hole state with energy $-E_g-\delta\varphi'-\hbar^2/2m_p(z_0')^2$ in a hole potential well of depth $-\delta\varphi'$ and size z_0', located at a distance R_t from the electron well; 3) tunneling annihilation of the captured electron and hole. Clearly, to realize the latter the energies of the electron and hole states must be equal, i.e.,

$$\delta\varphi'=\delta\varphi-E_g-\hbar^2/2m_nz_0^2-\hbar^2/2m_p(z_0')^2.$$

For simplicity we assume hereafter that the effective electron and hole masses are equal. It can then be assumed that the characteristic size of both fluctuations will be the same, $z_0=z_0'$.

We now write down equations, of almost the Shockley-Read type, which determine the change of the average occupation numbers in such a fluctuation pair:

$$\frac{\partial f}{\partial t}=\gamma_n[n(1-f)-n_1f]-\frac{1}{\tau_t}(f-f'),$$
$$\frac{\partial f'}{\partial t}=\gamma_p[p_1(1-f')-pf']-\frac{1}{\tau_t}(f'-f). \qquad (4)$$

Here

$$\tau_t\approx\frac{mz_0^2}{\hbar}\exp\left\{\frac{(mE_g)^{1/2}}{\hbar}R_t\right\}$$

is the characteristic tunneling time, n and p are the surface densities of the free electrons and holes, which are related by the Boltzmann equation with the corresponding densities in the electroneutral part of the substrate,

$$n_1=N_c\exp\left\{-\left(\delta\varphi-\frac{\hbar^2}{2mz_0^2}\right)\Big/T\right\},$$
$$p_1=N_v\exp\left\{-\left(E_g-\delta\varphi+\frac{\hbar^2}{2mz_0^2}\right)\Big/T\right\}$$

are the Shockley-Read parameters of the corresponding fluctuation states ($n_1p_1=n_i^2$).

Under stationary conditions ($\partial\{f,f'\}/\partial t=0$) we obtain for the number of electrons that recombine on such a binary fluctuation subsurface center per unit time,

$$\gamma_n[n(1-f)-n_1f]=\frac{np-n_i^2}{\tau_t(n+n_1)(p+p_1)+\gamma_p^{-1}(n+n_1)+\gamma_n^{-1}(p+p_1)}. \qquad (5)$$

The total flux of the electrons that recombine on the surface will be found by multiplying (5) by the average number of such binary fluctuation wells

$$\{\delta\varphi,\ \delta\varphi'\equiv\delta\varphi-E_g-\hbar^2/mz_0^2;\ z_0,\ R_t\}$$

per unit interface area, equal to

$$\frac{R_t}{z_0^3}\exp\left\{-\frac{K(z_0)\delta\varphi^2-2K(z_0,R_t)\delta\varphi\delta\varphi'+K(z_0)(\delta\varphi')^2}{2[K^2(z_0)-K^2(z_0,R_t)]}\right\}, \qquad (6)$$

and averaging the resultant expression over $\delta\varphi$. The Gaussian exponential, in which $K(z_0)\equiv K(z_0,z_0,0)$, and $K(z_0,R_t)\equiv K(z_0,z_0,R_t)$, is the joint probability of the existence, on the interface, of an electron potential well of depth $\delta\varphi$ and characteristic dimension z_0, at a distance R_t from which is located the hole well needed for the tunneling, with $\delta\varphi'=\delta\varphi-E_g-\hbar^2/mz_0^2$ and the same characteristic size. After simple transformations we obtain from (5), (6), and (1) for the effective surface-recombination rate

$$S(\varphi,z_0,R_t)=\frac{R_t}{z_0^3}\int d\left(\frac{\delta\varphi}{\Delta}\right)\frac{p_0}{\tau_t(n+n_1)(p+p_1)+\gamma_p^{-1}(n+n_1)+\gamma_n^{-1}(p+p_1)}$$
$$\times\exp\left\{-\frac{(\delta\varphi-E_g/2-\hbar^2/2mz_0^2)^2}{4\Delta^2\ln(R_c/z_0)}-\frac{(E_g+\hbar^2/mz_0^2)^2}{8\Delta^2\ln(R_t/4z_0)}\right\}. \qquad (7)$$

To obtain (7) we used the approximate relations

$$K(z_0)+K(z_0,R_t)\approx4\Delta^2\ln(R_c/z_0),$$
$$K(z_0)-K(z_0,R_t)\approx2\Delta^2\ln(R_t/4z_0),$$

a justified procedure so long as the characteristic tunneling length is $R_t\gg z_0$ and $R_c\gg R_t$. It will be verified below that these conditions are satisfied in the situations of interest to us. The Gaussian exponential in (7) shows that the most probable are tunneling binary fluctuations of equal amplitude ($\sim E_g/2$). We note also that the probability of realizing fluctuation pairs with small R_t, which are preferable for tunneling, is suppressed because the distribution of the random potential is correlated.

We now, in accord with the premises of the theory of optimal fluctuations,[5] obtain the extrema of (7) with respect to z_0 and R_t. Neglecting here the changes of the first term in

the argument of the exponential compared with the changes of the second, which has both a larger numerator and a smaller denominator, we obtain the nonlinear equations

$$\frac{1}{z_0^2}=\frac{1+z_0^{-2}}{4\ln(R_t/4z_0)}, \tag{8}$$

$$R_t=\frac{1}{8}\left(\frac{E_g}{\Delta}\right)^2\frac{(1+z_0^{-2})^2}{\ln^2(R_t/4z_0)}\left[\tau_t+\frac{1}{\gamma_n(n+n_1)}+\frac{1}{\gamma_p(p+p_1)}\right]\frac{1}{\tau_t}, \tag{9}$$

which determine the optimal z_0 and R_t (here and below z_0 and R_t are made dimensionless over the length $\hbar/(mE_g)^{1/2}$). In the square brackets of the right-hand side of (9), just as in the denominator (7), the tunneling time $\tau_t\approx(\hbar/E_g)z_0^2\exp R_t$ competes with the relatively long thermogeneration time $\tau_g\approx(\gamma_{n,p}n_i)^{-1}$. Depending on the ratio of the temperature and the characteristic fluctuation energy, two opposite situations are possible. In the first, which is realized at relatively high temperatures,[3] the tunneling time exceeds considerably the thermogeneration time τ_g, so that the latter can be neglected in (7) and (9) compared with τ_t. This means in fact that the electron and hole wells, which make up the considered fluctuation pairs, are in quasi-equilibrium with their bands, and the process that limits the recombination is the tunneling. In this case the system (8), (9) reduces to

$$z_0^2=4\ln\left(\frac{R_t^0}{4z_0}\right)-1, \quad R_t^0=2\left(\frac{E_g}{\Delta}\right)^2 z_0^{-4}, \tag{10}$$

and for the rate of the surface recombination we obtain the expression

$$S(\varphi)\approx\left(\frac{E_g}{\hbar}\right)^2\frac{m}{\hbar}\frac{p_0}{n_i^2}z_0^{-4}\exp\left\{-F\left(\frac{E_g}{\Delta}\right)\right\}\times\int d\left(\frac{\delta\varphi}{\Delta}\right)\frac{\exp\{-(\delta\varphi-{}^1/_2\tilde{E}_g)^2/4\Delta^2\ln(R_c/z_0)\}}{1+\operatorname{ch}\{(\varphi-\varphi_B+\delta\varphi-{}^1/_2\tilde{E}_g)/T\}}. \tag{11}$$

Here $\tilde{E}_g=E_g(1+z_0^{-2})$, and

$$F\left(\frac{E_g}{\Delta}\right)=\frac{1}{8}\left(\frac{\tilde{E}_g}{\Delta}\right)^2\left\{\ln^{-2}\left(\frac{R_t^0}{4z_0}\right)+\ln^{-1}\left(\frac{R_t^0}{4z_0}\right)\right\}, \tag{12}$$

where $z_0\equiv z_0(R_g/\Delta)$ and $E_t^0\equiv R_t^0(E_g/\Delta)$ is the solution of the system (10).

We note that in accord with the results of Ref. 1

$$2\Delta\ln(R_c/z_0)\approx\min\{\varphi+\mu, E_g-\varphi-\mu\}=E_g/2-|\varphi-\varphi_B|\approx E_g/2$$

and since the temperature $T\ll(E_g\Delta)^{1/2}$, at not too large values of $|\varphi-\varphi_B|<E_g\Delta/T$, i.e., in the vicinity of the maximum of $S(\varphi)$, the main contribution to the integral in (11) is made by the $\pm T$ vicinity of the minimum of the denominator of this expression, which consequently assumes in it the role of a δ-function. When integrating (11), its numerator can therefore be regarded as a slowly varying function, so that

$$S(\varphi)\approx\left(\frac{E_g}{\hbar}\right)^2\frac{m}{\hbar}\frac{p_0}{n_i^2}z_0^{-4}\exp\left\{-F\left(\frac{E_g}{\Delta}\right)\right\}\times\exp\{-(\varphi-\varphi_B)^2/\Delta(E_g-2|\varphi-\varphi_B|)\}. \tag{13}$$

Thus, at relatively high temperatures, when the tunneling is the decisive factor of the recombination process, the dependence of the rate of surface recombination on the average surface potential φ (the band bending) is described by a rather broad bell-shaped curve

$$\exp\{-(\varphi-\varphi_B)^2/\Delta(E_g-2|\varphi-\varphi_B|)\},$$

which is symmetric about the proper potential φ_B. As for the absolute values of the rate S, to determine them we must solve the system of nonlinear equations (1) and calculate the resultant dependence (12). It turned out that the asymptotic solutions of the system (10), which correspond to large or small values of the dimensionless parameter E_g/Δ, either take us outside the framework of the approximations used to analyze the problem (at $E_g/\Delta<1$) or are of no practical interest ($E_g/\Delta\gg1$, in which case negligibly small values of S are obtained). The nonlinear system (10) was therefore solved numerically. The solutions obtained in this case in the range of the parameter E_g/Δ of interest to us ($5<E_g/\Delta<20$) are close to the linear relations

$$z_0\approx2, \quad R_t^0\approx2E_g/\Delta, \quad F(E_g/\Delta)\approx4E_g/\Delta,$$

and this yields finally

$$S(\varphi)\approx\left(\frac{E_g}{\hbar}\right)^2\frac{m}{\hbar}\frac{p_0}{n_i^2}\exp\left\{-4\frac{E_g}{\Delta}-\frac{(\varphi-\varphi_B)^2}{\Delta(E_g-2|\varphi-\varphi_B|)}\right\}. \tag{14}$$

We consider now the opposite low temperature situation, which seems to us to be of greater practical importance, when the thermogeneration time is long enough and it follows from (9) that

$$R_t^0\approx\ln\frac{E_g}{\hbar\gamma N_c z_0^2}+\frac{E_g}{2T}, \quad \ln\frac{E_g}{\hbar\gamma N_c}=A\approx10, \tag{15}$$

which corresponds to equality of the thermogeneration and tunneling rates. In other words, all the fluctuation pairs with $R_t<R_t^0$ turn out in this case to be tunnel-coupled in the sense that the carriers captured in them annihilate by tunneling at practically equal probability, since the probability of their thermal ejection back into allowed bands is much lower than the tunneling probability. It is clear that this low-temperature situation is realized when the optimal tunneling length (15) exceeds the value $R_t^0\approx2E_g/\Delta$, corresponding to the solution of the system (10), i.e., when

$$A+E_g/2T>2E_g/\Delta. \tag{16}$$

It is this inequality which sets apart the considered low-temperature situation from the previously considered high-temperature one.

If (16) is satisfied it is necessary to substitute in expression (7) for the surface recombination the tunneling length (15) and the function $z_0(R_t^0)$ defined by (8). To find the latter it was again necessary to use numerical methods. All this yields in the upshot

$$S(\varphi)\approx\frac{E_g m}{\hbar^2}\frac{p_0}{n_i}(\gamma_n\gamma_p)^{1/2}\exp\left\{-\frac{1}{6}\left(\frac{E_g}{\Delta}\right)^2\ln^{-1}\left(1+\frac{E_g}{20T}\right)\right\}\times\int d\left(\frac{\delta\varphi}{\Delta}\right)\frac{\exp\{-(\delta\varphi-\tilde{E}_g/2)/\Delta E_g\}}{\operatorname{ch}\{(\varphi-\varphi_B-\alpha)/T\}+\operatorname{ch}\{(\delta\varphi-\tilde{E}_g/2+\alpha)/T\}}. \tag{17}$$

In the vicinity of the maximum of this expression $\varphi \sim \varphi_B + \alpha$ (we recall that $\alpha = \frac{1}{2}T\ln(\gamma_p/\gamma_n)$ the Gaussian exponential in the integral of (17) can also be regarded as a slowly varying function of $\phi\varphi$, and it is this which yields ultimately

$$S(\varphi) \approx \frac{E_g m}{\hbar^2}\frac{p_0}{n_i}(\gamma_n\gamma_p)^{1/2}\exp\left\{-\frac{1}{6}\left(\frac{E_g}{\Delta}\right)^2 \ln^{-1}\left(1+\frac{E_g}{20T}\right)\right\} \times \frac{\varphi-\varphi_B-\alpha}{T}\,\mathrm{sh}^{-1}\frac{\varphi-\varphi_B-\alpha}{T}. \quad (18)$$

The bell-shaped relation (18), which has a half-width of the order of $5T$ and is shifted by an amount α relative to the φ_B towards the inversion, is close both to the experimental $S(\varphi)$ dependences and to the form of the traditional expression (3) at $\varepsilon_t - \alpha < 1$. Comparison of (3) and (18) also shows that the actual result of the here-developed fluctuation model of surface recombination was the calculation of the effective density of the surface recombination centers

$$N_t = \frac{1}{z_0^2}\exp\left\{-\frac{1}{8}\left(\frac{E_g}{\Delta}\right)^2 \frac{(1+z_0^{-2})^2}{\ln(R_t/4z_0)}\right\} \approx \frac{E_g m}{\hbar^2}\exp\left\{-\frac{1}{6}\left(\frac{E_g}{\Delta}\right)^2 \ln^{-1}\left(1+\frac{E_g}{20T}\right)\right\} \quad (19)$$

as a function of the fluctuation energy Δ that characterizes the "quality" of the superconductor-insulator interface, which, according to the theory,[1] determines also the energy spectrum of the capture surface states (2).

We can now answer the question of the connection between the density of the surface states on the interface and the rate of surface recombination. The existence of this connection is beyond doubt, since expressions (14), (18), and (2) depend essentially on the characteristic energy Δ of the fluctuations. This connection, however, is not at all definite and is by far not reducible to a direct proportionality. The reason for this is obvious, since by far not all fluctuations with $\delta\varphi = \pm E_g/2$, which are optimal with respect to carrier capture, are also optimal for the recombination process. Contributing to the recombination flux is only a small fraction of these fluctuations, namely those located near an appreciable fluctuation of opposite sign.

This conclusion, which follows directly from the proposed fluctuation model of surface recombination, explains in particular why the spectra of the capture surface states practically never have near the middle of the forbidden band any specific peaks with which one could connect the traditional Shockley-Read mechanism of effective surface recombination. We therefore regard as incorrect also certain theoretical surface-recombination models[6,7] in which, roughly speaking, the surface states corresponding to continuous capture spectra are "assigned" specific capture recombination cross sections. The fluctuation model developed here leads to the opposite result: it is precisely the capture and recombination cross sections that are practically equal, while the effective surface densities of the corresponding centers differ strongly. Starting from this assertion, let us estimate the effective surface density (19) of the recombination centers for an Si–SiO_2 interface, using the capture coefficient γ determined experimentally, say, by the conductivity method,[8] $\gamma_n \approx \gamma_p \approx 10^{-9} - 10^{-8}$ cm^3·sec^{-1}. In this case ($E_g = 1.1$ eV) at $p = 10^{15}$ and $n_i = 10^{10}$ cm^{-3}, typical experimental values $S = 10$–100 cm·sec^{-1} are obtained at $N_t = 10^4 - 10^6$ cm^{-2}, which corresponds according to (19) to $\Delta \approx 0.09$ eV. This value of the fluctuation energy Δ, according to the surface-state theory,[1] corresponds to a built-in charge $\sigma = \Delta^2 x^2/\pi e^2 \approx 7\cdot 10^{12}$ cm^{-2} and a density of states at the minimum of the spectrum $N_{ss}(E_g/2) \approx 3\cdot 10^{12}$ cm^{-2}·eV^{-1}, values quite typical of so-called dirty Si–SiO_2 structures, on which the corresponding measurements of Refs. 9 and 10 were probably made. We note that for metal-oxide-semiconductor structures fabricated by the present state-of-the-art of silicon technology, in which $N_{ss}(E_g/2) \approx 10^{10}$ cm^{-2}·eV^{-1} (Ref. 2), and hence $\Delta \approx 0.04$ eV, Eqs. (14) and (18) give negligibly small values of S.

It must be noted, however, that in principle at small Δ (starting already with $\Delta < 0.07$ eV for Si–SiO_2 systems) the principal role in the recombination process should be assumed not by the considered Gaussian but by Poisson inherent-charge fluctuations, which are small-scale clusters of attracting centers that form quasi-atomic bound electron and hole states. In this case the effective density of the recombination centers is given not by (19) but by the Poisson expression

$$N_t = \frac{E_g m}{\hbar^2}\exp\left\{-4\left(\frac{E_g}{\varepsilon_0}\right)^{1/2}\ln\left(\frac{E_g^{1/2}\varepsilon_0^{1/2}}{\Delta^2}\right)\right\}, \quad \varepsilon_0 = \frac{me^4}{\hbar^2\varkappa^2}, \quad (20)$$

and this, of course, stabilizes considerably the $N_t(\Delta)$ dependence. This stabilization, however, is shown by estimates to take place on a level of exceedingly low $N_t < 10^{-4}$·cm^{-2}, so that the recombination on such Poisson fluctuations has no practical significance. Therefore the preceding statement that there is practically no surface recombination in high-grade Si–SiO_2 structures, remains in force.

In conclusion, a few words concerning the capture coefficients γ_n and γ_p, the ratio of which determines the shift of the maximum $S(\varphi)$. In the model proposed, both types of carrier are captured by attracting centers of approximately equal depth, $\sim E_g/2$, so that at first glance one can expect the corresponding capture coefficients to be close to each other. There is, however, an essential peculiarity that distinguishes between the capture of majority and minority carriers on surface states.

The point is that free minority carriers are "free" only with respect to tangential motions along the interface, while in the perpendicular direction they are almost as localized on this boundary as the bound states, owing to the action of the depleted-layer electric field that presses them towards the surface. Their capture (generation) on bound fluctuation surface states with binding energy ε defined relative to the central position of the conduction-band edge on the interface, i.e., relative to the percolation level, is therefore actually accompanied by release (absorption) of an energy ε. On the other hand, the motion of free majority carriers is infinite in all three coordinates, since the field of the depleted layer repels their interfaces. Moreover, when account is taken of the dimensions of the fluctuation potential wells in the perpendicular direction as a result of the peculiar quasi-Poole-Frenkel effect, the ionization energy of these states, i.e., the

energy barrier that prevents the bound majority carrier from going off to the substrate, turns out to be somewhat lower than the binding energy of this state, since the latter is also measured from the central position of the edge of the corresponding band on the interface.[11] This energy decrease $\delta\varepsilon$, according to an estimate in Ref. 11, amounts to several units of Δ.

In principle, this circumstance should be taken into account directly in Eqs. (4), by replacing in them p and p_1 the densities increased by a factor $\exp(\delta\varepsilon/T)$. If, however, this is not convenient for some reason, it is possible to use also the usual densities p and p_1 of the Shockley-Read theory, and the exponential can be assigned to the capture coefficient γ_p, as we must do in the present case. Consequently, other conditions being equal, the effective capture coefficient of the majority carriers (in our case, holes) should be $\exp(\delta\varepsilon/T)$ times larger than the capture coefficient of the minority carriers (electrons). This explains in fact, in our opinion, the experimentally observed exponential dependence of the ratio γ_p/γ_n on the reciprocal temperature.[3]

Naturally, in an n-type semiconductor the larger capture coefficient will be γ_n of the electrons, and the sign of α will be reversed. It follows therefore that regardless of the type of conductivity of the substrate, the position of the maximum of the surface-recombination rate will always be shifted away from the proper potential φ_B towards the inversion. The reverse picture would be observed if the surface recombination is via a monoenergetic surface state with a fully defined ratio of the electron and hole capture cross sections. Then, if the maximum of $S(\varphi)$ was shifted on the substrate having one type of conductivity, say, towards the inversion, then a shift of the maximum of $S(\varphi)$ towards the depletion should be observed on a substrate of the opposite type.

The foregoing constitutes that simple qualitative criterion with the aid of which one can determine whether the proposed fluctuation tunneling-thermogeneration mechanism of surface recombination is realized, or whether this recombination proceeds in accord with the traditional premises.

[1)]We shall use energy units for the potential and for the temperature, and assume for the sake of argument that the substrate has p-type conductivity.

[2)]$\hbar^2/2m_n z_0^2$ is the localization energy, which must be taken into account when determining the optimal size of the fluctuations.

[3)]The inequality that sets these situations apart is not obvious beforehand, and will therefore be given somewhat later.

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