Evolution of an impurity band during low-temperature application of a field to weakly compensated silicon with a high doping level

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(Submitted 4 July 1994; resubmitted 24 August 1994)
Pis'ma Zh. Eksp. Teor. Fiz. **60**, No. 6, 457–461 (25 September 1994)

When an electric field is applied to Si:B with a boron concentration of 10^{17-18} cm^{-3} at low temperatures, surface conduction channels form at relatively high voltages on the field electrode. The particular voltage varies with the doping level. When the Si surface becomes depleted of holes, the effect stems from the generation of a fluctuation potential due to impurity charge exchange. In the case of enrichment, in contrast, the effect stems from a filling of the upper Hubbard band under conditions of a hole-gas quantization. © *1994 American Institute of Physics.*

Low-temperature features of the formation of conduction channels at the surface of a semiconductor to which a field is applied are closely related to manifestations of a fluctuation potential, in particular, to a filling of localized states which arise at minima of the potential well.[1,2] Ideas regarding effects of a fluctuation potential have been developed primarily for an interface between a lightly doped semiconductor and an insulator whose potential fluctuates because of the random nature of the distribution of the charged centers in the insulator.[1,3,4] If the semiconductor is heavily doped, the effect of the low-temperature application of a field acquires a different physical nature, which is determined by the existence of an impurity band and the evolution of the structure of this band due to quantization of the hole gas and/or the generation of a fluctuation potential upon charge exchange of the dopant.

In the configuration for the application of a field, we studied thin (0.5-μm) layers of p-Si ($N_a \simeq 1\times10^{17}$ and 1×10^{18} cm^{-3}) fitted with two p^+ contacts. The layers were formed on a (100) n-Si substrate ($N_d \simeq 1\times10^{15}$ cm^{-3}) through ion implantation of boron. The polysilicon field electrode, with dimensions of 100×100 μm, was insulated from the p-Si by a layer of thermal oxide 620 Å thick. The procedure for fabricating the samples is described in Ref. 5.

We used the procedure of Ref. 6 to measure the electrical conductivity σ of the p layer as a function of the potential on the field electrode, V_g. The resulting curves (Fig. 1) demonstrate the onset of a surface enrichment channel ($V_g < V_{min}$) during application of the field. Under depletion conditions ($V_{min} < V_g < V_f$), a channel of a hopping transport

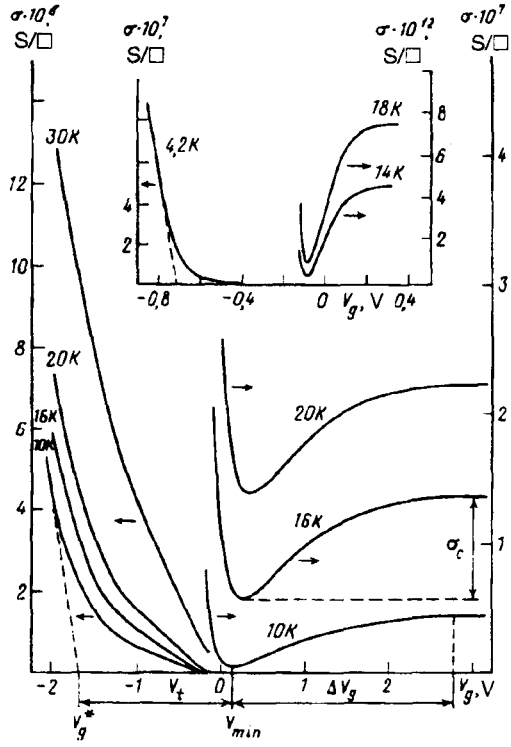

FIG. 1. Electrical conductivity of the p-Si layer as a function of the potential on the field electrode for various temperatures, for $N_a \simeq 1\times10^{18}$ cm^{-3} and 1×10^{17} cm^{-3} (in the inset).

due to the boron impurity arises. This transport is manifested over the temperature range[7] $T=6-300$ K. Here $V_{\min}$ is the flat-band voltage, which corresponds to the minimum of the $\sigma(V_g)=\sigma_{\min}$ curves,[7] and V_I is the inversion voltage. According to an estimate based on the Schottky approximation, this voltage has values of 3 and 10 V for $N_a \simeq 1\times10^{17}$ and 1×10^{18} cm^{-3}.

The surface hopping conductivity $\sigma_c=\sigma(V_g)-\sigma_{\min}$ initially increases with V_g and then goes onto a plateau. This behavior of $\sigma_c(V_g)$ was explained in Ref. 7 on the basis that the concentration of electrons at boron atoms increases until the boron level crosses the Fermi level. If we were to follow Ref. 7, we would expect that the $\sigma_c(V_g)$ curve would reach a plateau at a surface band curvature $\varphi_s \simeq \mu+\epsilon_c$, where $\mu=0.61q^2/(R_a\kappa)$ is the position of the Fermi level reckoned from the level of boron in the interior of the Si, R_a is the distance between impurities, κ is the dielectric constant of Si, $\epsilon_c \simeq E_F R_a$ is the activation energy for σ_c, and E_F is the electric field of the space-charge region formed by 2-complexes,[8] with a concentration N_d. Since the concentration of charges in the space-region is equal to N_d under the condition $\varphi_s<\mu$, while it is equal to N_a under the condition $\varphi_s>\mu$, the band curvature $\varphi_s \simeq \mu+\epsilon_c$ in the limit $T\to0$ corresponds to a surface electron density $n_s \simeq (\kappa/2\pi q)^{1/2}(\epsilon_c N_a+\mu N_d)^{1/2}$ (Ref. 1) and to a potential $V_{gs} \simeq 4\pi q n_s d_0/\kappa_0$ on the field electrode (κ_0 is the dielectric constant of SiO_2). For $N_a \simeq 1\times10^{17}$ and 1×10^{18} cm^{-3} we have $V_{gs} \simeq 0.16$ and 0.4 V, respectively. Actually (Fig. 1), the region in which the ϵ_c channel forms stretches out much further along the V_g axis: $\Delta V_g \simeq 0.5$ V ($N_a \simeq 1\times10^{17}$ cm^{-3}) and 2.5 V ($N_a \simeq 1\times10^{18}$ cm^{-3}).

This circumstance indicates a manifestation of a fluctuation potential, but this potential is not related to charges in the oxide, since ΔV_g increases with increasing N_a, while the charge density in the insulator for these samples, fabricated by a common procedure, is approximately constant at $n_t \simeq 4\times 10^{10}$ cm^{-2} (Ref. 5).

It is natural to associate this fluctuation potential with a change in the charge state of the boron, since we know[8] that when there are charges in a semiconductor, due to compensation, for example, the levels of the primary impurity have a distribution of energies and form an impurity band. In particular, with $N_a \simeq 1\times 10^{18}$ cm^{-3} and $N_d \simeq 1\times 10^{15}$ cm^{-3} the boron levels are localized in an energy band $W \simeq 1$ meV. The filling of boron atoms with electrons during application of a field will evidently give rise to a fluctuation potential; i.e., it will be accompanied by a broadening of the energy band W, which characterizes the boron impurity band near the maximum of its density. The value of σ_c will increase until the entire impurity band near the surface of the Si drops below the Fermi level, since in this case the number of states in the region in which the band intersects the Fermi level reaches a maximum (Fig. 2a).

Let us estimate the potential on the field electrode at which σ_c reaches the plateau, taking the broadening of the impurity band into account. Since W is limited from above by a value on the order of energy of the Coulomb interaction of neighboring boron atoms,[8] we assume $\varphi_s \simeq \mu + W_{\max}$, where $W_{\max} \sim a^2/(R_a \kappa)$. In particular, for $N_a \simeq 1\times 10^{18}$ cm^{-3} we have $W_{\max} \simeq 18$ meV $\gg \epsilon_c \simeq 1.6$ meV (Ref. 7). In other words, σ_c reaches the plateau at a greater band curvature under these conditions. Assuming that the distribution of impurity-band states in the band $W_{\max}$ is uniform, we find $n_s \simeq (\kappa/2\pi q)^{1/2}(2W_{\max}N_a + \mu N_d)^{1/2}$ and a field-electrode potential $V_{gs} \simeq 4\pi q n_s d_0/\kappa_0 \simeq 0.4$ V (1×10^{17} cm^{-3}) or 2.0 V (1×10^{18} cm^{-3}). Since this estimate is close to the values $\Delta V_g \simeq 0.5$ and 2.5 V (Fig. 1), the region in which the ϵ_c channel forms stretches out along the V_g axis because of the generation of the fluctuation potential as a result of filling of the boron impurities with electrons.

There is also the question of why ϵ_c is not the same as $W_{\max}$, since the relation $\epsilon_c \simeq W_{\max}$ usually holds.[8] The apparent reason is the nature of the fluctuation potential, which is a smooth potential: The screening radius of the fluctuation potential, which is determined in the absence of free charge carriers in the semiconductor by the thickness of the insulator,[4] is much greater than the distance between impurities, R_a. Accordingly, it is natural to represent the Si surface as a set of macroscopic regions (macroscopic at the scale R_a) with a uniform band curvature φ_s. In neighboring regions, the values of φ_s may vary over an interval of size $\sim W_{\max}$, but the energy barrier for hops of electrons will be approximately the same in all regions, since under the condition $\varphi_s \geqslant \mu$ it is determined by the value of μ and by the concentration of 2-complexes.[7] Figure 2 shows a qualitative picture of the situation here, for the example of two neighboring regions which differ in surface potential: An increase in the local value of φ_s causes the hopping-transport channel (the hatched region) to withdraw from the Si surface, but it does not affect the electric field in the space-charge region at the boundary separating the ionized and neutral impurity atoms.

The idea of a smooth induced fluctuation potential thus leads to an explanation of both the pronounced smearing of the region in which the ϵ_c channel forms and also the small activation energy for the hopping conductivity.

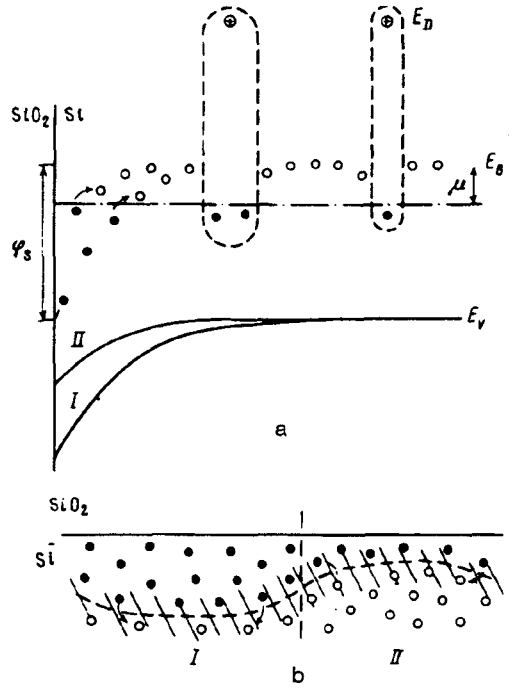

FIG. 2. Silicon surface layer under depletion conditions. a—Band diagram; b—spatial positions of ionized and neutral boron atoms in the plane perpendicular to the Si surface. Neighboring regions with different surface band curvature. The hatching represents a hopping-transport channel.

We turn now to the enrichment regime ($V_g < V_{\min}$), in which the $\sigma(V_g)$ curves exhibit an additional conduction threshold at low values of T : $V_t = V_{\min} - V_g^*$, where V_g^* is determined by extrapolating the linear part of the $\sigma(V_g)$ dependence, observed in the region of degeneracy of the hole gas, the V_g axis (Fig. 1). It would seem that under these conditions the boron would be mostly neutral, so the additional threshold could be caused only by a fluctuation potential induced by charges in the oxide.[4] Since V_t depends on N_a (Fig. 1), however, the particular features of the formation of the hole channel should be linked with other effects, namely a filling of states of an A^+ band (an upper Hubbard band[8]) and a quantization of the hole gas in the valence band. A necessary condition for the onset of a hole enrichment channel is that the Fermi level approach the top of a quantum subband[1] (Fig. 3). The band curvature in the space-charge layer formed during the filling of the A^+ band, i.e., $\delta\varphi = (2\pi q^2/\kappa) p_s^2/N_a$, must be the same as the energy of the quantum level,[1] $\epsilon_0 = (\hbar^2/2m)^{1/3}[(9\pi/8) q E_s)]^{2/3}$. Here p_s is the charge density in the A^+ band, and $E_s = (4\pi q/\kappa) p_s$ is the field at the Si surface. Equating $\delta\varphi$ to ϵ_0, we find $p_s \simeq 1.5\times 10^{11}$, 8.1×10^{11} cm^{-2}, and a threshold voltage $V_t = 4\pi q p_s d_0/\kappa_0 \simeq 0.42$, 2.2 V for $N_a \simeq 1\times 10^{17}$, 1×10^{18} cm^{-3}, respectively. These results agree with the experimental values of V_t (Fig. 1).

The curve of $\sigma(V_g)$ confirms the validity of our approach. The onset of a threshold voltage $V_t \simeq 2$ V (for the sample with $N_a \simeq 1\times 10^{18}$ cm^{-3}) requires a charge of density $n_t \simeq 8\times 10^{11}$ cm^{-2} in the oxide, which would be induced by a fluctuation potential with an energy scale $\Delta \simeq 20$ meV$\gg kT$. At this level we would expect an exponential dependence of σ on V_g in the below-threshold region.[2,4,9] Actually (Fig. 1), σ varies linearly with V_g at $V_g > -2$ V. This linear behavior is characteristic of manifestations of a weak

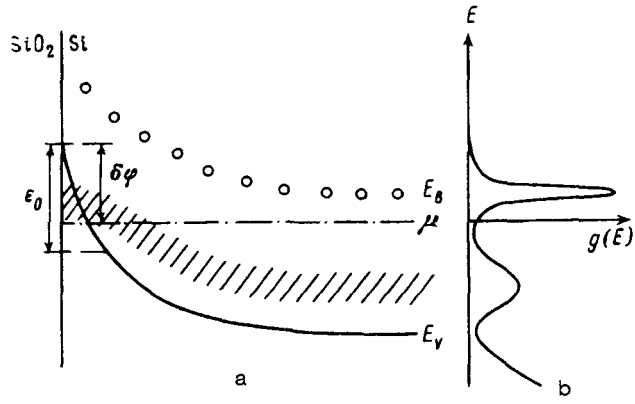

FIG. 3. a—Band diagram of the space-charge region in the enrichment regime; b—density of states in the interior of the Si. Dot-dashed line—Fermi level; solid line—potential of the space-charge region; dashed line—top of the hole quantum subband; hatched region—states of the A^+ band.

field effect[2,9] ($0.5<\Delta/kT<2$, $\Delta<1$ meV), which corresponds to $V_t<0.4$ V. On the other hand, at $N_a \geqslant 10^{17}$ cm^{-3} there is a band of delocalized A^+ states,[10] and a conductivity corresponding to these states may be predominant at low temperatures with a slight band curvature. Under these conditions the plot of $\sigma(V_g)$ below the threshold should be linear, with a slope determined by the mobility of the holes in the A^+ band. In the sample with $N_a \simeq 1\times10^{18}$ cm^{-3} at $T=6.3$ K, the effective hole mobility, $(d\sigma/dV_g)(4\pi d_0/\kappa_0)\simeq 11$ cm^2/V·s), is close to the hole mobility in the A^+ band [$\simeq 13$ cm^2/(V·s)] which was found in Ref. 10 from the temperature dependence of the ϵ_2 conductivity of Si:B with the same doping level.

We note in conclusion that the $\sigma(V_g)$ behavior is evidence that the quantization of the hole gas in the valence band affects the energy position of the A^+ states of boron. In this case the A^+ levels at the Si surface remain "shallow," as in the interior. In other words, they remain close to the top of the quantum subband, rather than following the potential of the space-charge region (Fig. 3). Otherwise, because of the high quantization energy ($\epsilon_0 \simeq 50$ meV for $N_a \simeq 1\times10^{18}$ cm^{-3}), the A^+-band conductivity would reach a plateau characteristic of a conductivity corresponding to the lower Hubbard band as V_g was varied.

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Translated by D. Parsons