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QUASIBREAKDOWN IN THE IMPURITY HUBBARD BAND SYSTEM OF NONCOMPENSATED SILICON

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It is discovered that in crystalline Silicon impurity conductivity abruptly increases with electric field E at $E > E_c$, where E_c - a certain threshold value of field. This increase -"the quasibreakdown" (QB) - is observed only in materials with extremely low compensation: $K < 10^{-3}$. The dependence $\sigma(E)$ in the QB region is approximated well enough by the expression $\ln\sigma \sim (-1/E)$. Weak magnetic field is able to supress QB completely. It is suggested that QB is a hopping conductivity through the localized states of upper Hubbard band tail, stimulated by electric field.

1. Lately the conductivity of doped by shallow impurities noncompensated Silicon has been intensively investigated in [1-4]. This conductivity has a number of very interesting peculiarities, which are connected mainly with the fact that the upper Hubbard band (UHB - D^--band or A^+-band in *n*- and *p*-type respectively) exerts decisive influence on the conductivity.

The present paper briefly describes the main results of the investigation noncompensated Silicon conductivity σ at helium temperatures in strong electric field E. A great number of samples of n- and p-type Si with impurity concentration $N \approx 10^{16} - 10^{17}\,\mathrm{cm}^{-3}$ and compensation $K \approx 10^{-5} - 10^{-3}$ were tested at temperatures $T = 4,2 - 18\,\mathrm{K}$.

2. The results of the measurements are illustrated in fig.1 which gives the profiles of $\sigma(E)$ for Si:B samples ($N \approx 6.5 \cdot 10^{16} cm^{-3}$, $K \simeq 10^{-4}$ - curve 1 and $N \approx 3.6 \cdot 10^{16} cm^{-3}$, $K = 1.5 \cdot 10^{-4}$ - curve *2*) obtained at $T = 4.2\,\mathrm{K}$. As one can see from the following discussion $\sigma(E)$ can be written down as

$$\sigma(E) = \sigma_T(E) + \sigma_E(E). \qquad (1)$$

The first term predominates in weak, the second - in strong E. σ_T weakly depends on E. On the contrary, σ_E sharply increases with E. This increase we will call quasibreakdown (QB). The critical field E_c, at which the QB begins, determined for sample 2 from the condition $\sigma_T(E_c) \approx \sigma_E(E_c)$, is roughly 180 V/cm. In sample 1 conductivity σ_T at 4.2 K is very small ($\sigma_T < 10^{-11}\mathrm{Ohm}^{-1} \cdot \mathrm{cm}^{-1}$) and we failed to measure it. One can see from curve 1 that for this sample $E_c(4.2\,\mathrm{K}) \lesssim 170\,\mathrm{V/cm}$. The conductivity $\sigma_T(E)$ was studied earlier in [1-3]. We will not consider σ_T here. It is necessary only to stress a fact essential for the following discussion: σ changes with magnetic field H very weakly, and this change is isotropic. (Here we always speak about weak fields $H \leq 10$ KOe). The subject of this paper is the σ_E - conductivity, which corresponds to the QB.

Let us point out the most important results:

- at $E > E_c$ (as at $E < E_c$) the Hall voltage V_H has failed to be measured: $V_H \approx 0$;
- E_c increases with K;

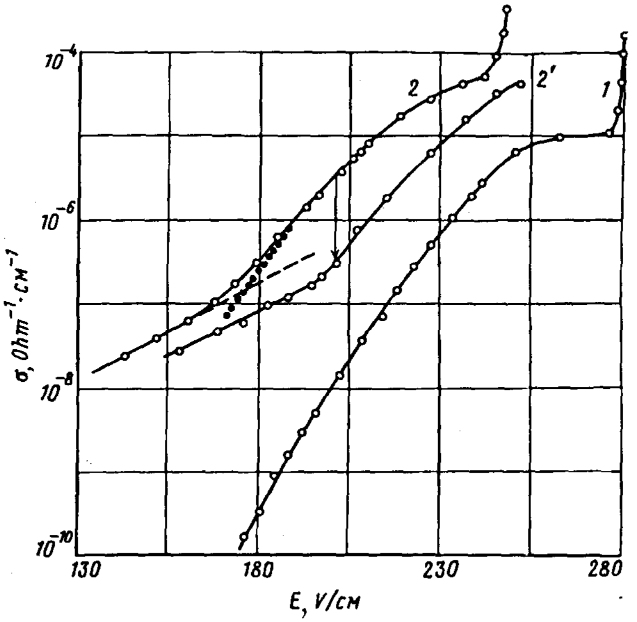

Fig.1. The dependence $\sigma(E)$ for Si:B at 4.2K for samples with N and K: *1* – $6.5 \cdot 10^{16}\,\mathrm{cm}^{-3}$, $K \approx 10^{-4}$; *2(2')* – $3.6 \cdot 10^{16}\mathrm{cm}^{-3}$, $K \approx 1.5 \cdot 10^{-4}$. *1* and *2* – $H = 0$; *2'* – $H = 10$KOe

– in transverse magnetic field QB moves to a stronger E-range: E_c increases with H. The curve 2' in fig.1 gives the $\sigma(E)$ in $H = 10$KOe for the sample 2. The vertical arrow in fig.1 shows the change of σ for the sample 2 at $E \approx 200$V/cm in the magnetic field $H \approx 10$KOe. The conductivity decreases by an order of magnitude: a great positive magnetoresistance (PMR) takes place. The longitudinal MR in such H is several times smaller.

Thus, the transverse H is able to suppress QB completely. Using this property of H, it is possible to separate σ_T and σ_E at $E \approx E_c$, where they are comparable. In fig.1 values of σ_T (shaded line) and σ_E (dotted line) thus obtained are shown.

3. Let us proceed to the discussion of the obtained results. First of all it is necessary to stress that QB is not an ordinary impurity breakdown, when free carriers appear. The fact that $V_H = 0$, when QB exists, is the evidence of their absence (holes in our case). The impurity breakdown (the vertical parts of the curves) arises at $E = E_b = 280$V/cm and 250V/cm for 1 and 2 samples respectively. At these E the Hall voltage appears. The field E_c is essentially less than E_b, and the dependence $\sigma(E)$ in QB region is by far smoother than that at the impurity breakdown. We must remind that E_b at $K \ll 1$ does not practically depend on K [5]. The field E_c essentially increases with K. At $K \approx 10^{-3}$ the field E_c reaches E_b and the electric field region in which QB can be observed vanishes.

This fact must be specially stressed. It explains why QB had not been discovered until materials with such small K appeared.

Thus QB represents an unknown before new phenomenon, characteristic of crystalline semiconductors with extremely small compensation.

4. At present there are theoretical and experimental studies [3, 4, 6] which evidence that in crystalline noncompensated semiconductors doped with shallow impurities the UHB – tail and the tail of lower Hubbard band (LHB – the ground

states band) overlap each other. At $T = 0$, the Fermi level ε_F lies in the region of overlapping tails. The density of unoccupied localized states rapidly increases with $\varepsilon - \varepsilon_F$. We suppose that the QB, discovered by us, is the variable hop conductivity through UHB-tail states, stimulated by electric field.

The nature of the phenomenon is the following. In the field E the Fermi level ε_F inclines. An electron with energy $\varepsilon < \varepsilon_F$ (in terms of n-type material) gets the opportunity to jump from under Fermi level into an unoccupied state of UHB - tail making an activationless hop. This hop and subsequent hops along unoccupied states give rise to electric current.

Such a mechanism was first proposed by Shklovskii [7]. In that paper the density of states is supposed to be constant. In this case the hops take place in the direct vicinity of the Fermi level. The dependence $\sigma(E)$ has the form: $\ln\sigma \sim (-E^{-1/4})$.

In our previous work [8] the theory of this phenomenon was developed for the case when the density of unoccupied states increases with ε rapidly enough.

The main results are as follows:

- if E is strong enough hops against the field predominate. The situation becomes one-dimensional;
- there is a certain level $\varepsilon_E(E)$ – the "transport level", along which an electron with energy ε_E hops keeping its average energy unchanged. Because of that electrons accumulate near the ε_E-level. On the other hand, the level ε_E lies essentially higher than ε_F. The density of states near ε_E is much greater and therefore the mean hop length is considerably less than that near ε_F. That is why the conductivity in strong E is completely determined by hops along ε_E-level. Thus, the stimulated conductivity can be considered as a multystep electric breakdown in the system of impurity Habbard bands of a crystal.

In [8] in order to obtain analytical expressions the one-dimensional density of unoccupied states is used in the form

$$g(\varepsilon) = g_F \exp((\varepsilon - \varepsilon_F)/\varepsilon_0) \tag{2}$$

where g_F – density of states at the Fermi level; ε_0 – a constant. The strong field condition is

$$\alpha(E) \equiv eE/g_F\varepsilon_0^2 \gg 1\,. \tag{3}$$

For ε_E and the typical hop length x_E the expressions obtained are:

$$\varepsilon_E = \varepsilon_F + \varepsilon_0 \ln\alpha, \qquad x_E = (\varepsilon_0/eE)\ln 2 \tag{4}$$

and for $\sigma(E)$:

$$\ln\sigma = -\beta(2\varepsilon_0/eEa)\,. \tag{5}$$

Here a – the localized state radius, $\beta = \beta(E) \simeq 1$ – the function which weakly (logarithmically) depends on E.

The origin of the dependence (5) is obvious. If E increases the level ε_E moves up to a region where $g(\varepsilon)$ is greater. The typical hop length x_E decreases in accordance with the second formula (4), and the hopping probability $\nu(\nu \sim \exp(-2x_E/a))$ increases according to the law: $\ln\nu \sim -1/E$.

In fig.2 the σ_E curves for samples 1 and 2 from fig.1 are drawn as functions of $1/E$. One can see that with a great degree of accuracy the function $f(1/E) \equiv \ln\sigma_E$ can be considered linear when σ_E changes by five (sample 1) and by three (sample 2) orders of magnitude, respectively. This result is a convincing argument in the favor of the model developed in [8].

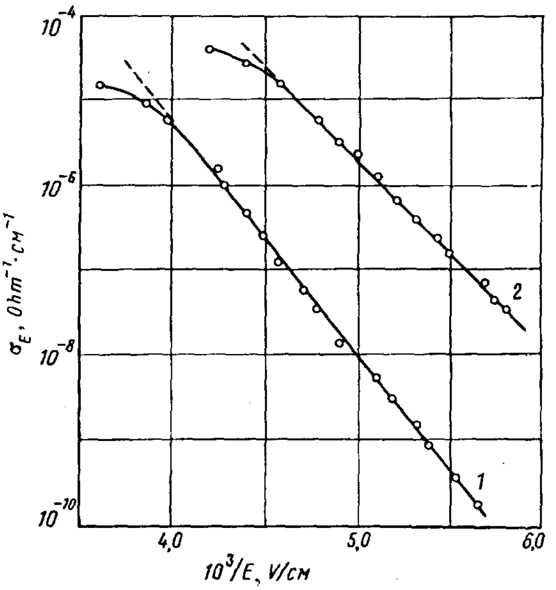

Fig.2. The σ_E curves for samples 1 and 2 of fig.1 are redrawn as function of $1/E$

It may seem strange, that the dependence $\ln\sigma_E \sim -1/E$ remains true throughout a very large interval of σ_E. Indeed, the special form (2) of density of states was used to obtain this dependence. However, it can be shown that for this dependence to exist the expression (2) must not be true in the whole interval $\varepsilon_F < \varepsilon < \varepsilon_E$, but only in that region $\Delta\varepsilon$, where the level ε_E lies at the given values of electric field. In our case $\Delta\varepsilon \lesssim \varepsilon_0$, while $\varepsilon_E - \varepsilon_F$ is equal to several ε_0.

At very strong E the dependence $\sigma(E)$ becomes weaker. This is apparently connected with the fact that ε_E is already in the region, where the dependence $g(\varepsilon)$ is smoother.

From the slope of the curves in fig.2 we evaluate ε_0, supposing $\beta = 1$ and $a = 10^{-6}cm$ (= radius of A^+-state in Si:B). For samples 1 and 2 we find it equal to ~ 4meV and ~ 3meV recpectively. The order of the values is the same as that of characteristic energy scale of the impurity band at $K \to 0$ (for example, ε_3 – the activation energy of hopping conductivity through LHB is of order of several meV).

The field E_c is defined by the condition $\alpha(E_c) = 1$. Indeed, at $\alpha \ll 1$ the level ε_E lies near ε_F: $\varepsilon_E - \varepsilon_F \ll \varepsilon_0$. At $\alpha \geq 1$ the level ε_E "comes off" ε_F and goes upwards to the region, where density of states is great. (The values of E_c, obtained from the experimental curves *1* above, in section two, are obviously slightly overestimated). Supposing $E_c \simeq 150$V/cm and $\varepsilon_0 \simeq 4$meV we find from the condition $\alpha(E) = 1$ that $g_F \simeq 10^4$meV$^{-1}\cdot$cm^{-1}.

On the other hand, the density of states (three dimensional) at the level ε_F in LHB is of the order of N_c/ε_3, where $N_c = KN$ – the concentration of the compensating impurity [9]. The corresponding one-dimensional density of states $N_c^{1/3}/\varepsilon_3$ is by an order of magnitude greater than g_F.

Thus, values ε_0 and g_F obtained from the analysis of experimental data appear reasonable.

Let us discuss now the effect of H on QB. In terms of [9] the fields $H \leq 10\,\mathrm{KOe}$ are weak for Si. In weak H an additional term $-\Delta\xi$ appears in the hopping conductivity exponent. To an accuracy of a factor close to 1:

$$\Delta\xi = \frac{r^3 d}{12\lambda^4}\,\overline{\sin^2\theta}. \tag{6}$$

Here r – typical hop length, $\lambda^2 = \hbar c/eH$ – magnetic length, θ – angle between H and hop direction. The line on the top means the averaging over directions of hops.

In small E hops' directions are isotropic: $\overline{\sin^2\theta} = 1/3$. $\Delta\xi$ does not depend on the angle between H and E. The anisotropy of MR is small and arises only because of the preexponential factor. Substituting $r \approx N^{-1/3}$ we get $\Delta\xi \ll 1$ at $H = 10\,\mathrm{KOe}$: MR is negligible.

In our case the transverse MR at 10 KOe is great: σ decreases by an order of magnitude. The longitudial MR is several times less. This is the evidence of the directional nature of the hopping movement. So, the condition of QB at $\mathrm{H} \perp \mathrm{E}$ implies $\Theta = \pi/2$ and $r \approx x_E$. At $E = 200\,\mathrm{V/cm}$ and $\varepsilon_0 \approx 3\,\mathrm{meV}$ the length $x_E \approx 10N^{-1/3}$. Then $\Delta\xi \approx 3$ and $\sigma(\mathrm{H})/\sigma(0) \approx 10^{-1}$, which agrees with the experiment. In these fields the dependence $\ln(\sigma(H)/\sigma(0)) \sim -H^2$ is observed, just as it should be.

Thus, the model of variable hopping length conductivity through D^--band tail states, stimulated by electric field, fairly explains the main pecularities of QB.

We suppose, that the $E_c(K)$ dependence is connected with decreasing of the probability for an electron to reach the ε_E level, when the concentration of the recombination centers increases.

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