Giant negative magnetoresistance accompanying a hopping conductivity in uncompensated silicon

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A negative magnetoresistance has been observed under hopping-conductivity conditions in silicon with a dopant concentration $N = 5\times10^{16}$–10^{17} cm^{-3} and a degree of compensation $K = 10^{-3}$–3×10^{-2}. This negative magnetoresistance reaches 100% at $H = 30$ kOe. It is suggested that the effect stems from a structural change in the dopant band in a magnetic field

We recently observed[1] a conductivity with a variable hopping length, of the Mott type, $\sigma = \sigma_M \sim \exp[-(T_0/T)^{1/4}]$ with an anomalously large positive magnetoresistance, in Si with very small K values and with values of N which are not very large ($K \leqslant 10^{-3}$, $N \leqslant 5\times10^{16}$ cm^{-3}; here and below, the data are given for Si:B). This conductivity is observed instead of a hopping conductivity with a constant activation energy ϵ_3 (σ_3 is the conductivity) and is therefore at odds with the standard interpretation.[2] It has been suggested that this conductivity with a variable hopping length, called a "high-temperature" conductivity in Ref. 1, and the large positive magnetoresistance (larger than usual by a factor up to 7–10!) stem from features of the dopant band of uncompensated samples. These features would in turn be due to a quantum overlap of states of neighboring centers. It has also been found that in samples with large values of N and K the high-temperature conductivity with a variable hopping length (VHL conductivity) gives way to a conductivity with a variable constant activation energy. In this letter we report a study of the effect of a field H on the resistance of this group of samples ($N = 5\times10^{16}$–10^{17} cm^{-3}, $K = 10^{-3} - 3\times10^{-2}$).

Figure 1 shows the relative change in the conductivity, $\delta\sigma_H/\sigma_0$ versus H at $T = 8$ K in various electric fields E for a Si:B sample with $N = 5.5\times10^{16}$ cm^{-3} and $K = 10^{-2}$. We see that there is a negative magnetoresistance. The ratio $\delta\sigma_H/\sigma_0$ goes through a maximum at a field $H = H_m(E)$ of 20–30 kOe. The value of $\delta\sigma_H/\sigma_0$ at the maximum is ~ 1. This result allows us to call the negative magnetoresistance a giant magnetoresistance, since it usually does not exceed 10%. With increasing E, the values of $\delta\sigma_H/\sigma_0$ and H_m increase. We wish to stress that in the case of the ordinary ϵ_3 conductivity there is a positive magnetoresistance. In a field $H = 30$ kOe it is on the order of 0.1.

Figure 2 shows curves of $\delta\sigma_H/\sigma_0$ versus $1/T$ for $H = H_m$ and various values of E. With a decrease in T, the curves have a maximum (T_m). With increasing E, the value of $\delta\sigma_H/\sigma_0$ at the maximum and T_m increase. At $T > T_m$ the ratio $\delta\sigma_H/\sigma_0 \sim \exp\Delta\epsilon/kT$, where the value $\Delta\epsilon$ (≈ 2.7 meV) does not depend on E and is the same for the five Si:B samples studied. For Si:B at approximately the same values of $N^{1/3}a_0$ (a_0 is the first Bohr radius) and K the curves are similar.

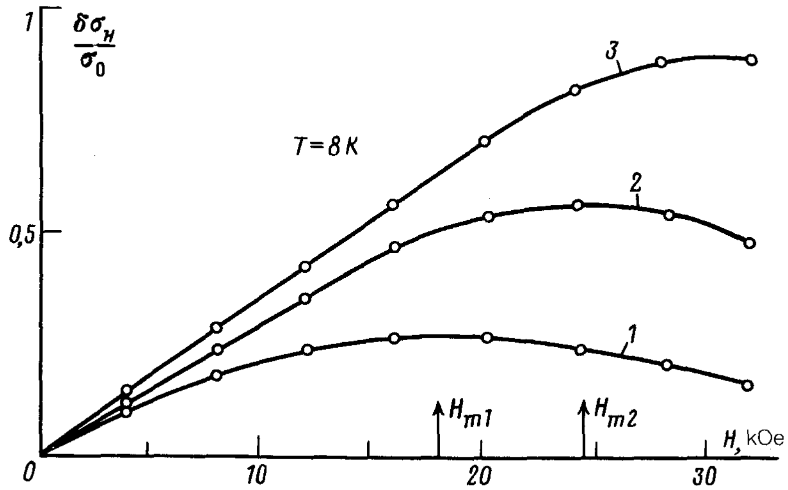

FIG. 1. Relative change in conductivity, $\delta\sigma_H/\sigma_0$ versus H at $T = 8$ K in several electric fields. 1—$E = 20$ V/cm; 2—100 V/cm; 3—180 V/cm.

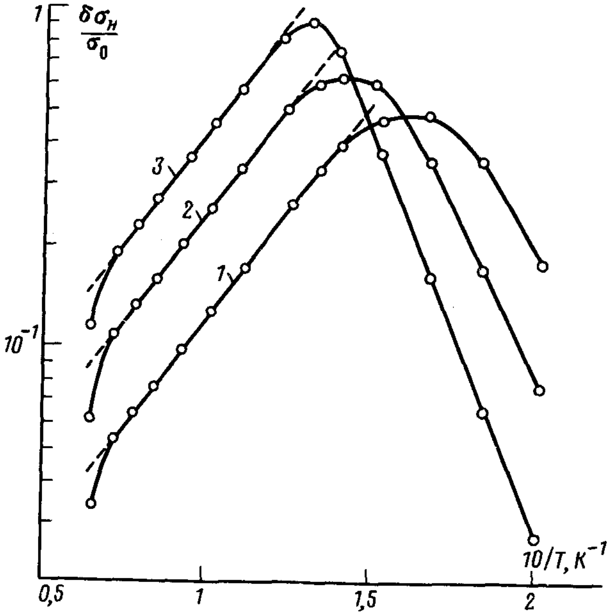

FIG. 2. Temperature dependence of $\delta\sigma(H_m)/\sigma_0$ in several electric fields. 1—$E = 20$ V/cm; 2—100 V/cm; 3—180 V/cm.

We will not go into a detailed discussion of these results here. We would like to offer a few comments regarding the nature of the giant negative magnetoresistance. In Ref. 1 it was noted that a pair of neutral hydrogen-like donors (the D_2 molecule; discussions for an n-type material) at a distance $R = R_m \simeq (3\text{–}4)\ a_0$ between them has a minimum energy of single ionization. This energy is lower than the ionization energy of an isolated center, ϵ_1, by an amount $\Delta\epsilon(R_m) \sim (0.06\text{–}0.07)\epsilon_1$. Consequently, the density of states in the dopant band should have, in addition to the basic peak $g_1(\epsilon)$ near the percolation level $\epsilon = -\epsilon_1$, and additional peak $g_2(\epsilon)$, with a maximum which lies a distance $\sim\Delta\epsilon(R_m)$ above this level (Fig. 3). If all the states in this peak are filled, all the D_2 molecules are neutral. If one state is vacant, then one molecule has lost an electron (has captured a vacancy) and has converted into D_2^+ ion. At $N \approx 5 \times 10^{16}\ \text{cm}^{-3}$ the density of states in the $g_2(\epsilon)$ peak is $\sim 0.05N$ and is considerably higher than the concentration of the dopant, NK.

We have attempted to relate the VHL conductivity and the large positive magnetoresistance to the circumstance that the Fermi level, near which the hops of variable length occur, lies near the $g_2(\epsilon)$ peak in the sample of Ref. 1. In the more heavily doped and compensated sample studied in the present experiments, the Fermi level is several kT's above the $g_2(\epsilon)$ peak. The presence of a constant activation energy ($\sim$4–5 meV) and several other properties are evidence that the hops occur near the percolation level. In this case the states in the $g_2(\epsilon)$ peak should serve as traps for carriers (vacancies). The depth of the trap is equal to $\Delta\epsilon(R_m)$. For Si:B ($\epsilon_1 = 45$ meV) we have $0.06\epsilon_1 = 2.7$ meV.

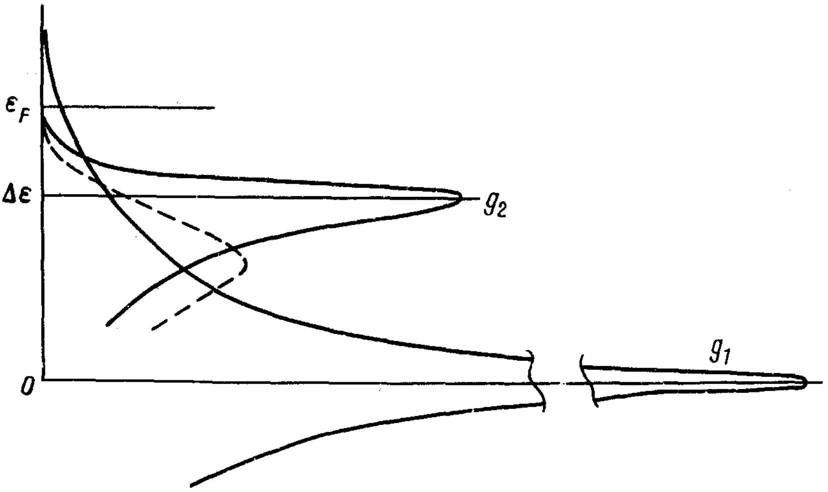

FIG. 3. Schematic diagram of the density of states. Here $g_1(\epsilon)$ is the main peak, and $g_2(\epsilon)$ is the additional peak. Solid line—$H = 0$; dashed line—$H = 30$ kOe.

Let us discuss the effect of H on $\Delta\epsilon(R_m)$. The energy $\Delta\epsilon(R)$ is the distance between the energy of the $D_2(\epsilon_{D_2})$ molecule and the energy of the system consisting of the $D_2^+(\epsilon_{D_2^+})$ ion plus the isolated neutral donor $D(\epsilon_D = -\epsilon_1)$ plus the electron at rest $(\epsilon = 0)$: $\Delta\epsilon(R) = \epsilon_{D_2}(R) - [\epsilon_{D_2^+} - \epsilon_1]$. At $R \approx (3\text{–}4)a_0$ the energy $\epsilon_{D_2}(R)$ is approximately equal to $-2\epsilon_1$ (Ref. 3). We therefore have $\Delta\epsilon(R) \approx -\epsilon_{D_2^+}(R) - \epsilon_1$. The energy $\epsilon_{D_2^+}$ should increase with increasing H. We can demonstrate this point by using the simplest calculation method: the LCAO method. In this method, the wave function ψ of the D_2^+ ion is written as the sum of atomic wave functions φ_a and φ_b of the a and b atoms. With $H \neq 0$, with the origin of coordinates at the nucleus of the a atom, we should write ψ as $\psi = \varphi_a + \varphi_b e^{i\chi}$, where $\chi = (e/2\hbar c)[\vec{H}\vec{R}]\vec{r}$, and the vector $\vec{R}$ runs from a to b (Ref. 2).

The factor $e^{i\chi}$ reduces that part of the electron energy charge density $e|\psi|^2$ which is associated with the overlap of the functions of different centers (the "overlap charge"[3]) by a factor of $\cos\chi$. As a result, the (negative!) potential energy of the electron and its total energy $\epsilon_{D_2^+}$ increase, while $\Delta\epsilon(R_m)$ decreases. The structure of the dopant band changes: The additional peak in the density of states, $g_2(\epsilon)$, descends, spreads out, and ultimately merges with the $g_1(\epsilon)$ peak. Vacancies move away from the trap and become conducting. Since the concentration of the traps which are of importance is $\sim g_2(-\epsilon_1 + \Delta\epsilon)kT > NK$, and since $\Delta\epsilon \approx 2.7$ meV, then at 8 K and $H = 0$ most of the vacancies are bound to traps. In a field H, the conductivity should increase substantially because of the increase in the concentration of conducting vacancies (Fig. 1).

The effect of H on the overlap charge is greatest in the region halfway between the atoms. The typical value of the phase is $|\chi| \sim R^2/\lambda_H^2$ $(\lambda_H^2 = \hbar c/eH)$. At $R = (3\text{–}4)\ a_0$, a significant negative magnetoresistance $(\chi \sim 1)$ can be observed at $\lambda_H^2 \gg a_0^2$. In this case the effect of H on an isolated donor can definitely be neglected. The equality $\lambda_H^2 = (4a_0)^2$ holds at $H \approx 50$ kOe ($a_0 = 23$ Å for Si:B).

A simple calculation shows that the activation energy observed in the presence of traps should be slightly greater than the distance between the Fermi level and the percolation level, and it should decrease with decreasing $\Delta\epsilon(R)$. Measurements confirm this interpretation: The activation energy decreases with increasing H, approaching its classical value $\epsilon_3 = e^2N^{1/3}/\kappa$, where κ is the permittivity.

We thus assume that the giant magnetoresistance and the conductivity observed in Ref. 1, with a variable hopping length with a large positive magnetoresistance, stem from dopant pairs with $R = (3\text{–}4)a_0$, which behave in different ways in samples with different values of N and K.

A significant increase in the negative magnetoresistance (Figs. 1 and 2) with E occurs in fields in which a negative deviation from an ohmic behavior is observed at $H = 0$ (Ref. 4). This effect stems from the dead ends of the critical subnetwork, which act as traps in strong fields E. In our measurements, the negative deviation from an ohmic behavior becomes less obvious with increasing H. This behavior suggest that the latter is associated with traps of two types: dead ends plus the "molecular" traps mentioned above, which intensify the effect and extend the range in which it is observed to lower values of T.

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