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Hole trapping by boron atoms in silicon at low temperatures

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Results are given of a study of the hole lifetime τ in Si:B as a function of the temperature T (2-18°K) and the trapping center concentration N (10^{13} - 10^{15} cm $^{-3}$). For $N < 10^{14}$ cm $^{-3}$, there was found to be a considerably weaker temperature dependence of τ at $T < 4^\circ\text{K}$. In samples with $N \sim 10^{15}$ cm $^{-3}$, τ was almost independent of the temperature below 10°K, and the dependence of τ on N was also much weaker. A qualitative interpretation of the experimental results is given, based on a simple model in which trapping is regarded as localization of a free carrier in a potential well attached to the impurity.

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It has been found¹⁻³ that at low temperatures hole trapping by boron atoms in silicon is not well described by the cascade theory of Lax,⁴ and the physical picture is considerably complicated by the possible trapping of holes by neutral boron atoms.^{2,3} This paper gives results of a study of the hole lifetime in boron-doped silicon as a function of the temperature and the trapping center concentration in samples with sufficient compensation ($K > 1\%$) to exclude any influence of hole trapping on neutral boron atoms. The experimental results are compared with the cascade trapping theory recently developed.^{5,6}

We determined the stationary hole lifetime τ . For this purpose, we measured the photo-Hall effect caused by a room temperature thermal background or by CO₂ laser radiation.⁷ In order to fix the absolute values of τ , we also measured the amplitude-frequency characteristics of the samples at 8-16°K.

Figures 1 through 3 show τ as a function of the temperature T and the trapping center concentration N ; in our experiments, the latter was almost equal to the concentration of the compensating donor impurities.⁷ The main features of the results are as follows.

1) The experimental temperature dependences of the lifetime throughout the ranges of T and N examined are considerably weaker than the relation $\tau \propto T^{3.5}$ predicted by Lax's theory.⁴

2) In samples with a low trapping center concentration $N \leq 10^{14}$ cm $^{-3}$ at $T < 4^\circ\text{K}$, there is a much weaker temperature dependence of τ , and $\tau \propto N^{-1}$.

3) When N increases, the weakening of the temperature dependence of τ begins at higher temperatures, and the dependence of τ on N is also considerably weakened. The value of τ is thus limited to 10^{-10} sec at least.

The anomalous behavior of the hole lifetime at $\tau \sim 10^{-10}$ sec, a value comparable with the hole energy relaxation time τ_E , was previously explained by a theory of hole heating by exciting radiation, on the supposition that the probability of hole trapping by an impurity center in interaction with acoustic phonons may exceed the probability of thermalization.⁸ In the theory,⁸ the influence of trapping on the photocarrier distribution function was taken into account by including in the transport equation a term $[-f(\epsilon)/\tau(\epsilon)]$, where $\tau(\epsilon) = \tau(kT)(\epsilon/kT)^n$ is the lifetime of carriers with kinetic energy ϵ . The quantity $\tau(kT)$ was taken

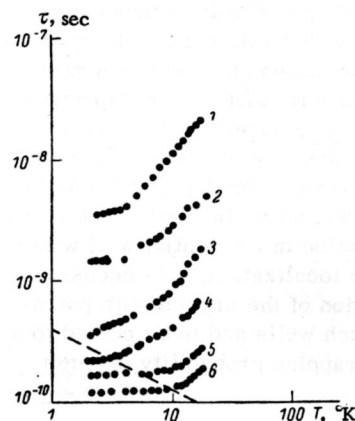


FIG. 1. Temperature dependences of photohole lifetime τ in boron-doped silicon for various trapping center concentrations, N (cm $^{-3}$): 1) $1 \cdot 10^{13}$; 2) $4.3 \cdot 10^{13}$; 3) $1 \cdot 10^{14}$; 4) $2.3 \cdot 10^{14}$; 5) $6.0 \cdot 10^{14}$; 6) $2.3 \cdot 10^{15}$. Dashed line: hole energy relaxation time for interaction with acoustic phonons, $\tau_E(kT)$; the points of intersection of the line with the experimental curves give the temperature T^* below which τ should be independent of T .

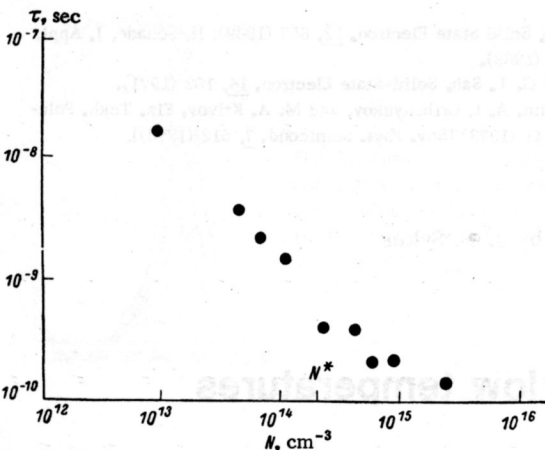


FIG. 2. Dependence of hole lifetime τ on trapping center concentration N at 13°K . $N^* \sim 2 \cdot 10^{14} \text{ cm}^{-3}$ is the value of N above which τ should vary less strongly with N at 13°K (Ref. 11).

equal to the equilibrium hole lifetime and obtained from experiment or from another theory, and the exponent n was used, in practice, as an adjustable parameter. It was then possible to account for the experimental results only semi-quantitatively. In the theory of photoheating,⁸⁻¹⁰ it was unjustifiably assumed that there might be a predominant emission of large acoustic phonons with energy $\hbar\omega > \varepsilon$ (trapping) relative to that of phonons with energy $\hbar\omega \ll \varepsilon$ with which the carriers most effectively interact. No allowance was made for the thermal release of carriers trapped at high excited states of the impurity center, which is an effective mechanism for Maxwellization of the distribution function when $\varepsilon \sim kT$. When τ was brought into the theory as a parameter, one could not take account of the overlap of excited states with binding energy $U \sim kT$. Moreover, it was not clear why the influence of overlap was estimated to begin just at $\tau \sim \tau_E(kT) \sim 10^{-10}$ sec in conditions where photoheating plays an important part. It was therefore necessary to construct a theory allowing for all these factors.

Such a theory has been developed.^{5,6,11} In it, carrier trapping and thermalization processes are regarded as a single continuous carrier energy relaxation process from the initial energy after photoexcitation $\varepsilon_i = \hbar\nu - \Delta E_i$ (where ΔE_i is the impurity ionization energy) to energies corresponding to localized impurity states. This process is governed by the interaction of carriers with acoustic phonons having energy $\hbar\omega \sim \sqrt{8ms^2\varepsilon} \ll \varepsilon$. In such a model, one can readily derive an expression for the carrier lifetime. Carrier capture at an attractive impurity center can be equated to carrier localization in a potential well with a certain depth U_C . For such localization, it is necessary for the carrier to be in a region of the crystal with potential energy U_C occupied by such wells and to be cooled to a kinetic energy $\varepsilon \lesssim U_C$. The trapping probability per unit time may then be written

$$\frac{1}{\tau} \sim A_r(U_C) \frac{1}{\tau_E(U_C)}, \quad (1)$$

where A_r is the probability that the carrier enters a region of space with potential energy U_C , and $1/\tau_E(U_C)$ is the probability of relaxation of the carrier kinetic energy

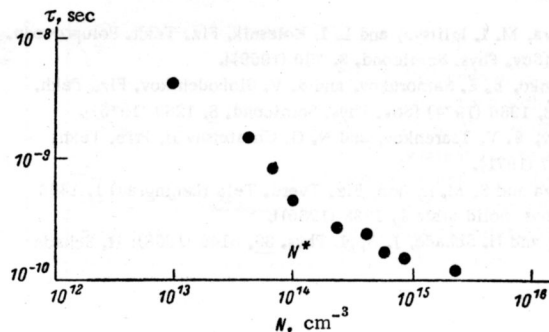


FIG. 3. Dependence of hole lifetime τ on trapping center concentration N at 4.2°K . $N^* \sim 10^{14} \text{ cm}^{-3}$ (Ref. 11).

to $\varepsilon \lesssim U_C$, per unit time.

When the trapping center concentration N is low, the carrier binding energy in the potential well is $U_C \sim kT$ (for small U , there is a large probability of reverse transfer of the trapped carrier into delocalized states).⁵ In this case, the characteristic dimension of the potential well $r_C \sim r_T = e^2/\kappa kT$ and the spatial probability $A_r \sim (4/3)\pi r_T^3 N$; for trapping in such a well, the carrier must cool to $\varepsilon \sim kT$ and $\tau_E(U_C) \sim \tau_E(kT)$. The result is

$$\frac{1}{\tau} \sim \frac{4}{3} \pi r_T^3 N \frac{1}{\tau_E(kT)}, \quad (2)$$

which agrees with the result of a rigorous theoretical treatment.⁵

The probability A_r is conveniently written as $A_r \sim (r_T/r_i)^3$, where $r_i \sim N^{-1/3}$ is the mean distance between trapping centers. At low impurity concentrations, $r_T \ll r_i$, $A_r \ll 1$ and $1/\tau$ increases with increasing N and decreasing temperature, since the region of space where the hole can be localized becomes larger: $A_r \propto NT^{-3}$. However, for sufficiently large $N \sim N^* \sim r_T^{-3}$ or low temperatures $T \sim T^* \sim \frac{1}{k} \left(\frac{e^2}{\kappa N^{-1/3}} \right)$, the characteristic dimension r_T of the potential well becomes comparable with the mean distance between trapping centers, and we have almost throughout the crystal a relief with depth $U_C \sim kT$. Then, the probability $A_r \rightarrow 1$, and it follows from Eq. (1) that the carrier lifetime is equal to the time for relaxation of the kinetic energy τ_E to $\varepsilon \sim kT$: $\tau \sim \tau_E(kT)$.

When N increases further, so does the depth of the potential relief due to the impurities (the carrier binding energy in the specific volume $r_i^3 \sim N^{-1}$ per impurity is $U_C \sim E_0 \sim e^2/\kappa r_i$): for $r_i < r_T$, the well depth $U_C > kT$. In this case, for localization the carrier need only be cooled to $\varepsilon \sim E_0 > kT$, i.e., the holes are trapped while hot and not yet thermalized: $\tau \sim \tau_E(E_0)$. Since $E_0 \propto N^{1/3}$, and $\tau_E \propto \varepsilon^{-1/2}$, the lifetime $\tau \sim \tau_E(E_0) \propto N^{-1/6}$ and is independent of the temperature. Thus, for $N > N^*$ and $T < T^*$, the dependence of the lifetime on the trapping center concentration should become much weaker, and the temperature dependence should disappear, which is in satisfactory agreement with experiment (Figs. 1-3).

Let us now consider the form of the distribution function for carriers that contribute to the photoconductivity. At sufficiently high values of ε , the energy of acoustic phonons that interact effectively with photocarriers is

$\hbar\omega \sim \sqrt{8ms^2\varepsilon} \gg kT$, and spontaneous emission of such phonons therefore predominates, the photocarrier distribution function being considerably different from the Boltzmann distribution: $f(\varepsilon) \propto \varepsilon^{-2}$. When $\varepsilon \rightarrow kT$, the energy relaxation becomes of the energy diffusion type (the phonon emission and absorption probabilities are of the same order), and the distribution function approaches the Boltzmann form $f(\varepsilon) \propto \exp(-\varepsilon/kT)$. At low trapping center concentrations $N < N^*$, according to Eq. (2), $\tau \gg \tau_E(kT)$, and the main bulk of the photocarriers undergo thermalization before being trapped. When the impurity concentration increases, $N > N^*$, at a given temperature, the depth of the potential relief due to charged impurities becomes greater, and therefore there is also an increase in the minimum kinetic energy of carriers that can contribute to the photoconductivity ($\varepsilon_{\min} \sim E_0 > kT$). The distribution function then has the non-Boltzmann form $f(\varepsilon) \sim \varepsilon^{-2}$ at all free photocarrier energies. Thus, the increase of N causes a heating of the photocarriers. This occurs, as is to be expected, with photocarrier lifetimes comparable with the characteristic times for establishment of their distribution function: $\tau \sim \tau_E(kT)$. However, in contrast to the theories,⁸⁻¹⁰ the photocarrier heating is due not to the predominance of trapping over thermalization but to the localization of carriers with kinetic energy ε below $E_0 > kT$ in the potential relief due to the random distribution of trapping centers.

The theory⁶ also gives an explanation of the weakened temperature dependence of τ when $\tau \gg \tau_E(kT)$ in samples with a low trapping center concentration. This weakening must occur when $kT \ll ms^2$; in silicon, $ms^2 \sim 3^\circ K$ for holes. The reason is that, when $kT \ll ms^2$, the bulk of the carriers with energy $\varepsilon \sim kT$ cannot be trapped into impurity states with binding energy $U \sim kT$, since a carrier with energy $\varepsilon < ms^2$, is prevented by the conservation laws from emitting an acoustic phonon. In this case, to be trapped, the carrier must approach the impurity center to within a distance $r_S \sim e^2/\kappa ms^2 < r_T$ in a region with potential energy $U_C \sim ms^2$. In this region, holes are accelerated by the attractive potential of the impurity, and their kinetic energy $\varepsilon \geq ms^2$. It then becomes possible for phonons to be emitted, i.e., for energy relaxation to occur below $\varepsilon = ms^2$, resulting in trapping. The hole trapping probability per unit time in this case may be expressed similarly to Eq. (1) if we take the depth of the potential well $U_C \sim ms^2$.

However, in contrast to Eq. (1), A_T must take account of the higher density of states in the potential wells than in the rest of the crystal. The density of states $\rho \propto \sqrt{\varepsilon}$, and in the region with potential energy $U \sim ms^2$ (where the kinetic energy $\varepsilon \sim ms^2 \gg kT$) the density of states is increased by a factor $\sqrt{ms^2/kT}$. Consequently, $A_T \sim \frac{4}{3} \pi r_S^3 \cdot \sqrt{ms^2/kT} N$ and

$$\frac{1}{\tau} \sim \frac{4}{3} \pi r_S^3 \sqrt{\frac{ms^2}{kT}} N \frac{1}{\tau_s(ms^2)}. \quad (3)$$

It is seen that, when $ms^2 \gg kT$, the temperature dependence is considerably weakened ($\tau \propto T^{-0.5}$); this is mainly because, in that case, the size r_S of the potential well is independent of the temperature. The approximate expression (3) for the carrier trapping probability is in satisfactory agreement with the results of the exact calculation.⁶

The temperature dependence of the lifetime may also become weaker with falling temperature when $\tau \gg \tau_E$ because some of the trapping centers are coupled into dipoles.¹¹ A detailed quantitative comparison of the experimental results with the theory has been given.¹¹

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