

# Spin-dependent recombination on dislocation dangling bonds in silicon

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Spin-dependent recombination of free carriers via dislocation dangling bonds is investigated as a function of the temperature and of the light power in magnetic fields 0.04, 3.3, and 12.5 kOe. A model of the effect is proposed on the basis of an analysis of the obtained data. The model makes use of the concept of recombination via the dangling bonds, with preliminary capture of the carriers by intermediate shallow levels assumed to be due to the deformation potential of the dislocation.

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## 1. INTRODUCTION

It can be regarded as established by now that dislocations in silicon plastically deformed at  $T \leq 720$  °C contain chains of dangling bonds which produce an EPR signal and cause deep donor and acceptor states in the forbidden band.<sup>1,2,3</sup> The onset of these levels (or narrow bands) is due to the possibility of capture, by the dangling bond, of a hole or of an additional electron. Since the number of such states is quite large ( $N_{\text{DDB}} > 10^{16}$  cm<sup>-3</sup> at a strain  $\epsilon = 1.5\text{--}2\%$ ) and they have large capture cross sections for both electrons and holes,<sup>4</sup> one can expect them to make the decisive contribution to the carrier recombination. Since an electron or hole can be captured by a dangling bond only in the singlet spin state, it is quite probable that the recombination rate depends on the spin state of the dangling dislocation bonds (DDB).

The simplest method of investigating spin-dependent recombination (SDR) is to saturate the EPR signal that equalizes the populations of the Zeeman levels, and to observe under these conditions the changes in the recombination rates. Such an effect was observed by Lepin on surface centers in silicon.<sup>5</sup> This effect was later observed by us on dislocations in silicon at helium temperatures,<sup>6</sup> and by Figitelski and Wosinski<sup>7</sup> in the 300–100 K range on deformed silicon. The SDR effect was later observed by Solomon *et al.* in amorphous silicon. All the experiments except in Ref. 6 were performed in the range 300–77 K, and in a magnetic field of the order of 3 kOe.

The simplest variant of an explanation of SDR in the case of dislocations is the following: the applied constant magnetic field  $H_0$  polarizes the spins and the free carriers as well as the DDB electrons. Since capture can take place only in the singlet state, the probability of which is proportional to

$$\pi_s = \frac{1}{4} - \langle \hat{S}_e \hat{S}_{\text{DDB}} \rangle,$$

the average capture probability, neglecting capture processes with spin flip, is

$$W_c = \frac{1}{4} (1 - p_e P_{\text{DDB}}) W_{c0}. \quad (1)$$

Here  $p_e$  and  $P_{\text{DDB}}$  are the equilibrium spin polarizations of the electrons and of the DDB ( $p \sim H_0/T$ ). A resonant microwave field superheats the DDB spin system until  $P_{\text{DDB}}$  van-

ishes. As a result, a change should be observed in the recombination rate  $R$ , with  $\Delta R/R \approx p_e P_{\text{DDB}} \sim H_0^2/T^2$  (Ref. 5). At  $T = 300$  K and  $H_0 \approx 3$  kOe we should have  $\Delta R/R \ll p_e P_{\text{DDB}} \approx 10^{-6}$ . The value of  $\Delta\rho/\rho$  observed in all experiments, however, exceeds by several times the calculated  $p_e P_{\text{DDB}}$ . Several models were proposed to explain the large value of the SDR, but there is still no unambiguous interpretation of the observed effect in the case of dislocations in silicon. In Ref. 4 was proposed a model for the production of polarons via interaction of DDB with the captured electron, while in Ref. 8 a ferromagnetic exchange interaction between a neighboring DDB was suggested. Both models led to a large value of the effect on account of the increase of  $P_{\text{DDB}}$ . It was shown<sup>9</sup> that the exchange interaction between the DDB should be antiferromagnetic, and a model was proposed in which the SDR is due to resonant heating of the phonon system or of the exchange reservoir<sup>10</sup> in EPR.

In Ref. 11, finally, a model was discussed in which the electron and the hole are captured by closely located traps without an intrinsic spin. In this case only singlet pairs can recombine, and the lifetime of the triplet pairs are determined only by the thermal ionization, which leads to their accumulation. If the microwave field is capable of transforming the triplet state into a singlet state, SDR will be observed, and the magnitude of the effect can reach 10% and is independent in first-order approximation of the field  $H_0$ . It was reported in the same paper<sup>11</sup> that SDR in amorphous silicon, measured at 300 K and at microwave frequencies 9.3 and 1.9 GHz, turned out to be of the same order ( $\Delta\rho/\rho \approx 10^{-4}$ ), in agreement with the proposed mechanism.

Later<sup>12</sup> measurements of SDR on deformed silicon at frequencies 9.3 and 2.4 GHz and at 300 K likewise yielded equal values of the effect, close to<sup>11</sup> ( $\Delta\rho/\rho \approx 10^{-4}$ ), and the SDR had approximately the same width and the same g-factor as in Ref. 13. The results of Ref. 12 were explained within the framework of the model proposed in Ref. 11.

When discussing these results, it seems important to us to call attention to the fact that plastic deformation of the silicon produces, beside the DDB, also certain paramagnetic centers whose parameters (line width, g-factor, spin-lattice relaxation time) differ from those of DDB and agree with the parameters of the EPR centers in amorphous silicon.<sup>14</sup> When the samples are annealed at temperatures above

650 °C, the EPR spectrum of the DDB vanishes (the activation energy of the process is  $\sim 2$  eV), and all that is left is the EPR line from those "amorphous" centers whose number is usually not more than 7–10% of the initial DDB concentration even in strongly deformed samples.<sup>15</sup> It is not excluded that plastic deformation produces microscopic regions of the amorphous phase or separately broken the bonds, surrounded by a strongly distorted lattice and similar to the EPR centers in *a*-Si. We note that in Refs. 7, 8, and 12 the characteristics of the SDR also agreed with the parameters of the EPR signal in *a*-Si (width 6 Oe,  $g = 2.004$ – $2.005$ ). We therefore assume that the samples investigated in the cited references were without DDB and the SDR was similar to the SDR in amorphous silicon.

The purpose of the present study was to investigate SDR on DDB in silicon in various magnetic fields at low temperature, with an aim at studying the mechanism of this effect.

## 2. SAMPLES AND MEASUREMENT PROCEDURE

We used samples of single-crystal *p*-type silicon ( $10^{13}$  cm $^{-3}$  of boron) grown by crucible-less zone melting in vacuum. The samples were plastically deformed at 700 °C in an argon atmosphere by compression along  $\langle 110 \rangle$ . The sample preparation procedure is described in detail in Ref. 16. The deformation time was 4–5 min. The degree of deformation (strain) of the samples was 2–2.5%, corresponding to a dislocation density  $(1\text{--}3) \times 10^9$  cm $^{-2}$  and to a DDB density  $N_{\text{DDB}} \approx (2\text{--}3) \times 10^{16}$  cm $^{-3}$ , as determined by EPR at  $T > 50$  K, (Ref. 2), i.e., the average distance between the DDB along the dislocations did not exceed 5–7 Å. The Fermi level in the non-illuminated samples at  $T < 200$  K lies in the region of  $E_v + 0.42$  eV (Ref. 17), therefore the dark conductivity at  $T < 100$  K is negligibly small. The sample resistance was measured by a four-contact method, the sample dimensions were  $2 \times 2 \times 7$  mm when measured at 9 and 110 GHz and  $1 \times 1 \times 5$  mm at 36 GHz.

When working at 9 and 36 GHz the sample was placed in the antinode of a microwave stainless-steel cavity (wall thickness 0.3 mm) with a copper coating on the outside. Modulating coils were placed on the cavity and were used to apply to the sample an alternating field of frequency up to 1 kHz parallel to the constant external field. In the measurements in the 110 MHz range the cavity was replaced by a coiled wire. The sample was illuminated through a filter of pure silicon 2 mm thick by a miniature incandescent lamp mounted on the cavity.

The sample conductivity was replaced by measuring the voltage drop between potential contacts with direct current flowing through the sample. The voltage was measured with an electrometric amplifier having an input resistance up to  $10^{14}$  Ω. The amplified voltage, past the analog-digital converter, was read with a minicomputer that controlled the experiment in real time. The experimental procedure was the following: the dependence of the sample resistance of the magnetic field was recorded in the region of the resonance conditions for EPR with the microwave power on and off. The difference between the functions yielded the influence of

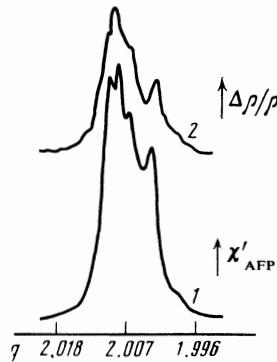


FIG. 1. DDB EPR spectrum,  $\chi'_{\text{AFP}}$ , and the SDR spectrum ( $H_1 = 0.02$  Oe) at  $T = 1.4$  K;  $H_0 \parallel [111]$ ;  $H_0 = 3.3$  kOe.

the microwave field on the sample conductivity. To improve the signal/noise ratio the procedure was repeated a number of times and the SDR signal was accumulated.

## 3. EXPERIMENTAL RESULTS

We describe first the results obtained in the 9.3 GHz range, i.e., at a static magnetic field of approximately 3.3 kOe. Figure 1 shows the EPR spectrum of the DDB recorded in the adiabatic fast passage (AFP) regime,<sup>18</sup> and the SDR spectrum recorded at microwave field values  $H_1$  of the order of 0.02 Oe. The spectra were obtained at  $T = 1.4$  K and with weak illumination corresponding to a sample conductivity  $\sigma \approx 10^{-10}$  Ω $^{-1}$ ·cm $^{-1}$ . It is seen that the sample resistance increases on passing through magnetic resonance corresponding to DDB (i.e., the recombination probability increases), and the SDR spectrum is similar in shape and in characteristics to the DDB EPR spectrum.

As shown earlier<sup>2,18</sup> the EPR spectrum of the DDB is inhomogeneously broadened and consists of individual spin packets spaced 0.6–0.8 Oe apart in a 3.3 kOe field. The inhomogeneous broadening is due in the main to the scatter of the  $g$  factors, so that the spectrum width increases in proportion to the magnetic field. Indeed, it was found that at an orientation  $H_0 \parallel [111]$  the width of the EPR spectrum of the DDB is of the order of 15.5 Oe in a 3.3 kOe field, 38 Oe in a 12.5 kOe field, and according to the SDR data, of the order of 7–8 Oe in a 0.04 kOe field.

It follows from these data that the spectrum broadening can be described by the empirical relation

$$\Delta H \approx 7.5 + (\Delta g/g) H_0, \quad \Delta g \approx 5 \cdot 10^{-3}.$$

At not too high a microwave power, the only DDB saturated are those for which resonance conditions are satisfied, and the observed value of the SDR should be less than the true value corresponding to saturation of the entire spectrum, even if the saturation conditions

$$\gamma^2 H_1^2 \tau_{1,\text{eff}} \tau_{2,\text{eff}} \gg 1$$

are satisfied for the individual spin packets.

To know the total width of the effect, we have the total value of the effect, we have used modulation of the magnetic field  $H_M \sin \omega_M t$ , such that  $2H_M > \Delta H$  and  $\omega_M \tau_1 \gg 1$ . Here  $H_M$  and  $\omega_M$  are respectively the amplitude and frequency of

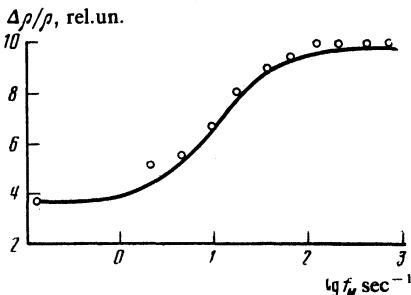


FIG. 2. Dependence of the SDR on the modulation frequency of the constant magnetic field. Solid curve—calculation by formula (2).

the modulation. In this case it becomes possible to saturate the EPR signal of all the spin packets. Indeed, when this condition is satisfied the magnetic moments of the spin packets stay half the time in an inverted state and the projection of the moment on the magnetic field is on the average zero. The use of this method uncovers a possibility of determining the characteristic SDR time, whence the dependence of  $\Delta\rho/\rho$  on  $\omega_M$  is found. In fact, regardless of the SDR mechanism, it is possible to introduce a time  $\tau_1^*$  during which the system "remembers" that a definite spin packet was saturated. If it is assumed that the contribution to the SDR from the  $i$ -th packet after being acted upon by the microwave field decreases like

$$(\Delta\rho/\rho)_i \sim \exp(-t/\tau_1^*),$$

it is easy to obtain the dependence of the quantity  $(\Delta\rho/\rho)f_M$  on the modulation frequency. In the general case this quantity depends on  $H_1, \Delta H, H_M$ , and on the ratio of  $\omega_M$  and  $\tau_1^*$ , and the expression is quite unwieldy. However, at  $2H_M \gg \Delta H$  and  $\gamma^2 H_1^2 \tau_1^* \tau_2^* \gg 1$ , where  $\tau_2^* \approx (2\gamma H_M)^{-1}$ , the expression takes the simpler form

$$(\Delta\rho/\rho)_{f_M} = A + 2Bf_M\tau_1^*[1 - \exp(-1/2\tau_1^*f_M)], \quad (2)$$

where

$$\begin{aligned} f_M &= \omega_M/2\pi, \quad A = (\Delta\rho/\rho)_{f_M=0}, \\ B &= (\Delta\rho/\rho)_{f_M \rightarrow \infty} - (\Delta\rho/\rho)_{f_M=0}. \end{aligned}$$

Figure 2 shows by way of example the dependence of  $\Delta\rho/\rho$  on  $f_M$ , obtained at  $T = 1.4$  K, and the calculated curve [Eq. (2)];  $\tau_1^*$  and  $B$  are determined by a best least-squared fit to the experiment.

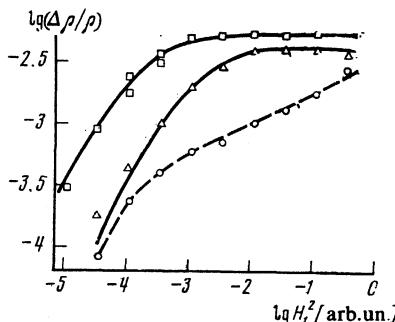


FIG. 4. Dependence of the SDR on the microwave power at  $T = 1.4$  K;  $\square - \rho = 3 \cdot 10^8 \Omega \cdot \text{cm}, f_M \gg (\tau_1^*)^{-1}$ ;  $\circ - \rho = 5 \cdot 10^8 \Omega \cdot \text{cm}, f_M = 0$ ;  $\triangle - \rho = 5 \cdot 10^9 \Omega \cdot \text{cm}$ , and  $f_M \gg (\tau_1^*)^{-1}$ . The solid curves were calculated from formula (6).

Figure 3(a) shows the dependence of  $\tau_1^*$  on the illumination level at  $T = 1.4$  K. The same figure shows the values of  $\tau_1$  measured by pulsed saturation of the EPR signal of the DDB. The EPR signal was detected in the adiabatic fast passage regime at a modulation frequency 600 Hz and a saturating-pulse duration 3 sec. Figure 3(b) shows the dependence of the EPR signal  $\chi'$  on the illumination level. We note that when the illumination is turned off  $\chi'$  and  $\tau_1$  are restored to their dark values. The restoration time of  $\chi'$  did not exceed the spin-lattice relaxation time in darkness.

Figure 4 shows the experimental dependences of the SDR  $\Delta\rho/\rho$  on the amplitude  $H_1$  of the microwave field, obtained at  $T = 1.4$  at a modulation frequency  $f_M > 1/\tau_1^*$ . Also shown is the  $\Delta\rho/\rho$  dependence without field modulation.

Figure 5 shows the temperature dependences of  $\tau_1^*$  and  $\Delta\rho/\rho$ . In the temperature region  $T > 35$  K, the value of  $\Delta\rho/\rho$  corresponds to saturation of the entire EPR spectrum of the DDB, i.e., the condition  $f_M \tau_1^* \gtrsim 1$  was satisfied, corresponding to the plateau on the plots of  $\Delta\rho/\rho$  against  $f_M$  (Fig. 2), and the microwave field  $H_1$  was also strong enough to maintain the effect constant when  $H_1$  changed slightly (this corresponds to the plateau on Fig. 4). Figure 5(a) (curve 1) shows the values of  $\tau_1$  obtained by pulsed saturation of the EPR spectrum of the DDB in Ref. 2. It is important that the values of  $\tau_1$  and  $\tau_1^*$  differ greatly.

The next result was that an increase of the magnetic field  $H_0$  from 3.3 to 12.5 kOe did not increase  $\Delta\rho/\rho$  by  $\sim 16$  times, as expected, but even decreased it somewhat.

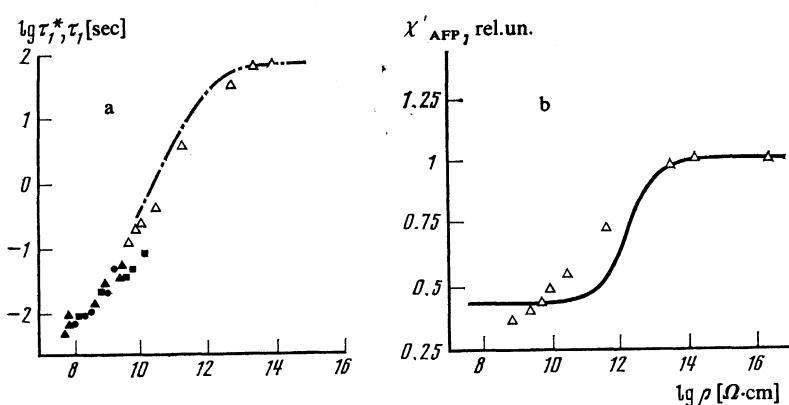


FIG. 3. a)  $\blacktriangle, \blacksquare, \bullet$  relaxation times  $\tau_1^*$  of SDR for different samples,  $\triangle$ —spin-lattice relaxation time  $\tau_1$ ,  $T = 1.4$  K; b)  $\triangle$ —dependence of the DDB, EPR signal  $\chi'_\text{APP}$  at  $T = 1.4$  K on the sample resistivity  $\rho$ . The solid curve was calculated from formula (10).

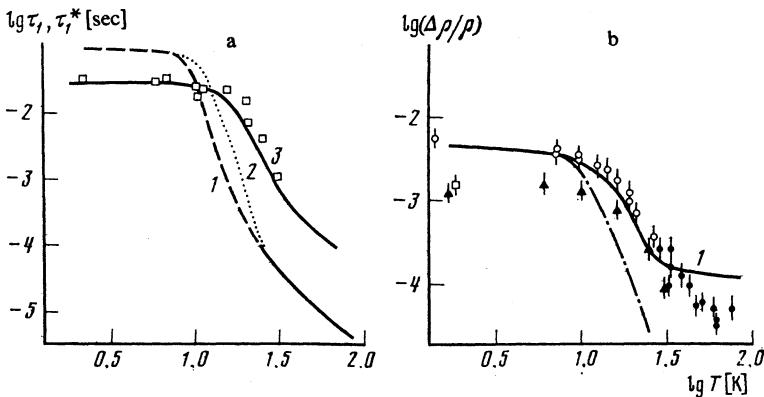


FIG. 5. a)  $\square$ —temperature dependence of  $\tau_1^*$ , curve 3—calculated dependence of  $\tau_1^*$  ( $W_c$  and  $W_D$  were calculated from formula (11)); curves 1—spin-lattice relaxation time  $\tau_1$ , dashed curve—values of  $\tau_1$  used in the calculation of the quantities  $\Delta\rho/\rho$ ;  $\rho = 3 \cdot 10^9 \Omega\text{-cm}$ . b)  $\square$ — $H_0 = 40$  Oe;  $\nabla$ — $H_0 = 12$  kOe;  $\bullet, \circ$ — $H_0 = 3.3$  kOe ( $\circ$ — $f_M > (\tau_1^*)^{-1}, \frac{1}{4} \gamma^2 H_1^2 \tau_{\text{eff}} \tau_2^* > 1$ );  $\rho = 3 \cdot 10^9 \Omega\text{-cm}$ . Curve 1—calculation by formula (6) at  $W_c$  and  $W_D$  from formula (11), values of  $\tau_1$  from curve 2 of Fig. 5a; dash-dot—value of  $\Delta\rho/\rho$  under the assumption  $W_c = \text{const} = 63 \text{ sec}^{-1}$  and  $\tau_1$  from the formula of Ref. 2.

For a more unambiguous choice of the model we have measured the SDR in a field  $H_0 \sim 39$  Oe (frequency 110 MHz) and obtained approximately the same value as in the 12 kOe field. Thus, the effect is independent, in first-order approximation, of  $H_0$  in the range from 40 Oe to 12.5 kOe. It is important that at the same  $\rho$  and  $T$  the value of  $\tau_1^*$  is likewise independent of  $H_0$ .

The values of  $\Delta\rho/\rho$  at 12.5 kOe (frequency 35 GHz) and 0.04 kOe (110 MHz) can be seen in Fig. 5(b). Finally, Fig. 6 shows the values of  $(\Delta\rho/\rho)$  for total saturation of the EPR spectrum of DDB as a function of  $\tau_1^*$ , obtained at  $T = 1.4$  K for different illumination conditions, i.e., different values of  $\rho$  [see Fig. 3(a)]. It should be noted that the maximum value of the effect varied somewhat from sample to sample, depending on the strain.

#### 4. DISCUSSION OF RESULTS

Thus, on passing through the paramagnetic resonance condition for the DDB in plastically deformed silicon samples, a decrease of the photoconductivity is observed. This can be interpreted as an increase of the rate  $R$  of the recombination of the electrons and holes on the DDB. It is important that the magnitude of the effect  $\Delta R/R$  is practically

independent of the static magnetic field applied to the sample (at least in the range from 39 to  $12.5 \times 10^3$  Oe), and the characteristic time of the effect  $\tau_1^*$ , during which the recombination “remembers” the action of the resonant microwave field on the DDB is much longer than the spin-lattice relaxation time  $\tau_1$  of the DDB (see Fig. 5), and also depends weakly on the magnetic field  $H_0$ . The magnitude of the effect  $\Delta\rho/\rho \approx \Delta R/R$  remains practically unchanged when the temperature is raised from 1.3 to 10 K, after which it decreases rapidly;  $\tau_1^*$  behaves similarly with changing temperature, but a change of the illumination level affects  $\tau_1^*$  much more strongly than it does  $\Delta R/R$  (Figs. 3 and 6).

We shall attempt below to choose an SDR model capable of explaining these facts and of understanding, at least qualitatively, the observed temperature dependence of  $\Delta\rho/\rho$  and  $\tau_1^*$ . In addition, we must discuss the causes of the strong change of the quantities  $\tau_1$  and  $\tau_1^*$  with change in the illumination condition. This model should also agree with the known experimental facts concerning the energy spectrum of the DDB.<sup>1,3,17</sup>

Let us discuss once more briefly the main existing models of the spin-dependent recombination. The first type of model is based on the spin dependence of the capture of free electrons (or holes) by centers having an intrinsic spin in the absence of an additional electron (e.g., by the DDB). It is assumed that the capture can occur only in a singlet final state ( $S = 0$ ). If capture with simultaneous spin flip is neglected, it is easy to obtain for the capture probability expression (1). In the paramagnetic case we have  $p \propto H_0/T$ , where  $H_0$  is the static magnetic field,  $T$  is the temperature of the spin system. At paramagnetic resonance for the DDB, the spin system of the DDB absorbs energy from the microwave field  $H_1$ , and if the field is strong enough total equalization of the populations of the Zeeman levels of the DDB becomes possible, corresponding to vanishing of  $P_{\text{DDB}}$ . One should observe in this case an increase in the rate  $R$  of carrier capture by the DDB, with  $\Delta R/R \approx p_e P_{\text{DDB}}$ . In the case of paramagnetism we should thus have

$$\Delta\rho/\rho \approx \Delta R/R \propto H_0^2/T^2,$$

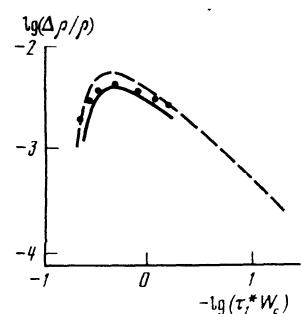


FIG. 6. Dependence of  $\Delta\rho/\rho$  on  $\tau_1^*$  at  $T = 1.4$  K. ●—experimental points. The curves were calculated from Eq. (6); solid curves  $N = 8$ ,  $W_c = 63 \text{ sec}^{-1}$ , with account taken of  $\tau_1$ ; when account is taken of the exchange field  $H_{ee}$ , the same curve corresponds to  $N = 20$ , the dashed curve— $N = 9$ ,  $W_c = 63 \text{ sec}^{-1}$ ,  $\alpha = 10^{-5}$ .

which disagrees with the experimental data both in functional dependence and in absolute value.

The assumption that a ferromagnetic interaction exists in the DDB system on account of direct exchange<sup>8</sup> or on account of formation of ferromagnetic polarons when the DDB interact with the captured electrons<sup>4</sup>, makes it possible to improve somewhat the agreement with experiment, i.e., to increase the calculated value of the effect via increasing  $P_{\text{DDB}}$  and weaken the dependence on the magnetic field at sufficiently strong fields via saturation of  $P_{\text{DDB}}$ . However, a dependence on the magnetic field of the type  $\Delta R / R \propto H_0$  should be observed just the same, owing to the polarization of the free carriers. In addition, the assumption of direct ferromagnetic exchange<sup>8</sup> does not agree with the EPR data.<sup>2,18</sup> Thus, in this way one can hardly obtain agreement with experiment. The models of the second type are based on allowance for the fact that when captured by deep centers, such as DDB, the electrons should give up to the lattice a rather high energy. One of the ways of capturing by a deep level due to the DDB is the Lax cascade process with excitation of local vibrational modes of the dislocation core. These local modes should play a substantial role also in the spin-lattice relaxation of the DDB and it is this which apparently leads to the observed anomalously weak temperature dependence of  $\tau_1$ , observed in Ref. 2. Upon saturation of the EPR signal of the DDB, the system of the localized phonons may turn out to be significantly overheated relative to the remaining lattice, because of the effective interaction with the spin system of the DDB. This in turn, can lead to an increase of the capture probability and to recombination of the carriers. Such a model of the SDR was proposed in Refs. 9 and 19.

In Ref. 10 is considered an analogous possibility, connected with the cascade process of magnon radiation and with the superheating of the exchange reservoir upon saturation of the magnetic resonance in the chains of exchange-coupled DDB (an antiferromagnetic interaction between the neighboring DDB), which does not contradict the EPR data<sup>2,18</sup> was assumed). In both cases the magnitude of the effect is described by the expression

$$\frac{\Delta R}{R} \approx \alpha \left( \frac{\tau_1^*}{\tau_1} \right) \frac{\chi_0 H_0^2}{CT}, \quad (3)$$

where  $\tau_1^*$  is the temperature-relaxation time of the localized phonon reservoir (or of the exchange reservoir), i.e., a parameter that characterizes the coupling of this reservoir with the lattice;  $C$  is the heat capacity of this reservoir;  $\chi_0$  is the magnetic susceptibility of the spin lattice,  $H_0$  is the magnetic field,  $\tau_1$  is the relaxation time of the homogeneous precession excited upon magnetic resonance, and

$$\alpha = T \left[ \frac{\partial (W_e)}{\partial T} \right]_T \frac{1}{W_e},$$

where  $c$  is the electron-capture probability. We note that in this model the characteristic SDR time is determined by  $\tau_1^*$ , which can differ from  $\tau_1$ . The case  $\tau_1^* > \tau_1$  corresponds to the "phonon bottleneck."

Generally speaking, one can attempt to attribute the independence of  $\Delta R / R$  of  $H_0$  to the exotic dependence of  $\tau_1$  and  $\tau_1^*$  on  $H_0$ , but this is not very likely. Thus, it is apparently

impossible to explain the experimental results on SDR with the aid models of the second type.

In Ref. 11 was proposed a fundamentally different SDR model, which differs substantially from the first type in that the electrons and holes are first captured by certain closely lying centers that have no intrinsic spin (and this process is spin-independent), yet the probability of further recombination, which due to the possibility of tunneling between the centers, is spin dependent. SDR can be observed in this situation because only singlet electron-hole pairs can recombine, and the lifetime of the triplet pairs is long enough to make their thermal ionization possible, after which the electron excited into the conduction band can again participate in the conduction. If the microwave field can mix effectively at resonance the singlet and triplet states, an increase will be observed in the recombination rate, and the effect in first-order approximation is independent of the applied static field  $H_0$ . We believe this idea to be quite fruitful and shall use it to construct our model of SDR on dislocations in silicon. For this purpose it is convenient to reformulate the model as applied to this case.

#### 4.1 SDR model on DDB

According to Refs. 1, 17, and 3, the main part of the energy spectrum of the electronic states of the DDB consists of two narrow bands,  $E_1 \approx E_c + 0.38$  eV and  $E_2 \approx E_c + 0.67$  eV. The states  $E_1$  correspond to the DDB electrons themselves or to holes captured by DDB. The states  $E_2$  correspond to electrons captured by DDB in the singlet state. We assume that the DDB system corresponds to a one-dimensional Mott-Hubbard dielectric with narrow bands.<sup>17</sup> In addition to the bands  $E_1$  and  $E_2$  there exist levels connected with different defects on dislocations,<sup>1,3</sup> but their density is low compared with the DDB at approximately the same capture cross sections, so that when discussing the SDR effects we shall not consider them. Besides the deep levels connected with the DDB, there can obviously exist slower one-dimensional bands for holes and electrons, due to the presence of deformation potential near the dislocation cores, which leads to a local change of the width of the forbidden band.<sup>20</sup> The calculated depth of these levels is not more than 0.05–0.1 eV. It is important that they must be spatially separated to some degree from the DDB (see Fig. 7). Let the energies of the electrons and holes in such bands be  $E_{ed}$  and  $E_{hd}$ . We assume that the probability of carrier capture into the bands  $E_{ed}$  and  $E_{hd}$  is much higher than the probability of direct

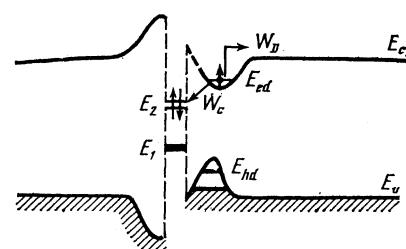


FIG. 7. Dislocation-level scheme (see explanation in text).

capture into the bands  $E_1$  and  $E_2$  (first because  $E_{ed}$  and  $E_{hd}$  are shallow, and second because of the larger number of states). The recombination will then proceed as follows: the electrons and holes are captured into the bands  $E_{ed}$  and  $E_{hd}$ , after which the transitions  $E_{ed} \rightarrow E_2$  and  $E_{hd} \rightarrow E_1$  take place. Next, since the electrons in  $E_2$  and the holes in  $E_1$  can move along the dislocations, they arrive at one dangling bond, which corresponds to their recombination  $E_1-E_2$ . Since the  $E_1$  and  $E_2$  bands are deep enough, the thermal activation of the carriers captured by them in the  $E_c$  and  $E_v$  at  $T < 100$  K can be neglected, i.e., a carrier captured in  $E_1$  or  $E_2$  is assumed to be lost, and sooner or later recombines. Since the situation for the holes and electrons is symmetrical, we consider for the sake of argument electron capture.

We shall show that the SDR can be due to the spin-dependent character of the transition of the electron from  $E_{ed}$  into  $E_2$ , i.e., to a dangling bond.

We consider a finite isolated chain of DDB, consisting of  $N$  spins. The probability of electron capture from  $E_{ed}$  by this chain (into the  $E_2$  band) is  $W_s W_c$ , where  $W_c$  is the probability of the transition of an electron from  $E_{ed}$  into  $E_2$  (per dangling bond in the singlet state) and  $W_s$  is the probability that the electron-DDB pair has (prior to the transition) oppositely directed spins (i.e., forms a singlet configuration). If the  $g$ -factors of the DDB and of the electron in  $E_{ed}$  differ somewhat, the spin precession in the field  $H_0$  causes the probability  $W_s$  to contain a term that oscillates with frequency  $|g_e - g_{DDB}| \gamma H_0$ . If this frequency is much higher than  $W_c$ , we can use a certain mean value  $W_s$ . Let the angle between  $H_0$  and the electron spin be  $\theta$ , then, as is well known, the probability of the state  $+1/2$  is

$$\cos^2(\theta/2) = (1 + \cos \theta)/2,$$

and of  $-1/2$ :

$$\sin^2(\theta/2) = (1 - \cos \theta)/2,$$

or, putting  $\cos \theta = p$ , we obtain respectively  $(1 + p)/2$  and  $(1 - p)/2$ .

Since the electron can move along the chain, i.e., it can be captured by any of the DDB and there exists in the chain an effective exchange of spins between the DDB, it is important for us to have the average probability, for the given chain, of observing any spin of the DDB in the states  $+1/2$  or  $-1/2$ . It is a rather complicated task to calculate rigorously this probability, but one can estimate quite reliably the effect for the case  $N \gg 1$ , if it is assumed that each of the DDB spins is in a "pure state"  $+1/2$  or  $-1/2$ . The problem of finding the average spin projection for a given chain (i.e., of its polarization), reduces to the problem of placing  $N$  particles in  $2N$  states. The probability that the polarization of this chain is

$$\bar{p}_2 = (N_+ - N_-)/(N_+ + N_-),$$

where  $N_+$  is the number of spins in the state  $+1/2$  and  $N_-$  is the number in the state  $-1/2$ , can be easily shown to be

$$W(\bar{p}_2) = (N!)^4 / (2N!) [(N - N_+)! (N_+!)^2].$$

We neglect here the influence of the external field  $H_0$  on the polarization. If we have an electron in  $E_{ed}$  with polariza-

tion  $p_1$  and the polarization of the DDB chain is  $\bar{p}_2$ , the probability of capturing an electron in the band  $E_2$ , i.e., in singlet states, with one of the DDB, is

$$\begin{aligned} W_c W_s(p_1; \bar{p}_2) &= {}^1/{}_8 W_c [(1 + p_1)(1 - \bar{p}_2) + (1 - p_1)(1 + \bar{p}_2)] \\ &= {}^1/{}_4 W_c (1 - p_1 \bar{p}_2). \end{aligned} \quad (4)$$

Introducing the DDB spin-flip probability  $W_f$  (on account of the spin-lattice relaxation and spin-spin interactions with other chains, or on account of the microwave field at resonance), and the probability of activating an electron from  $E_{ed}$  to the percolation level and its departure from the chain ( $W_D$ ), we have for the number of pairs  $n(p_1; \bar{p}_2)$  consisting of an electron in  $E_{ed}$  and a DDB chain, with given  $p_1$  and  $\bar{p}_2$ , the following balance equation:

$$\frac{dn(p_1; \bar{p}_2)}{dt} \approx \frac{GW(\bar{p}_2)}{2}$$

$$-n(p_1; \bar{p}_2) [W_D + W_s(p_1; \bar{p}_2) W_c + W_f] + N(p_1; -\bar{p}_2) W_f,$$

whence

$$n(p_1; \bar{p}_2) \approx \frac{2GW(\bar{p}_2)/W_c}{4\lambda + 1 - p_1 \bar{p}_2 + 8\alpha p_1 \bar{p}_2 / (8\alpha + 4\lambda + p_1 \bar{p}_2 + 1)}, \quad (5)$$

where  $\lambda = W_D/W_c$ ;  $\alpha = W_f/W_c$ ;  $G$  is the rate of electron generation by the light. From this we can easily obtain the recombination rate

$$R = \sum_{N_+=0}^N \int_{-1}^1 n(p_1; \bar{p}_2) \left( \frac{W_c}{4} \right) (1 - p_1 \bar{p}_2) dp_1 \quad (6)$$

and the average lifetime of the electron in  $E_{ed}$ :

$$\tau_1 = \frac{1}{G} \sum_{N_+=0}^N \int_{-1}^1 n(p_1; \bar{p}_2) dp_1. \quad (7)$$

Upon saturation of the EPR of the DDB we increase the probability of the DDB spin flips on account of the microwave field. At  $H_1 \rightarrow \infty$  we have

$$\alpha = W f_{mw} / W_c \rightarrow \infty,$$

which leads to an increase of the probability of the transition  $E_{ed} \rightarrow E_2$  of those electrons which made up triplet configurations with the DDB and could not be captured by them. As a result, the average lifetime  $\tau_1^*$  decreases somewhat and the recombination rate increases. It is important that after summing over  $p_1$  and  $\bar{p}_2$  there is no magnetic-field dependence in first-order approximation.

Since the condition that the number of electrons in the conduction band be stationary can be written in the form

$$nW_s - R = 0,$$

where  $R$  is the rate of an electron capture in  $E_2$  followed by their recombination,  $n$  is the density of the free electrons, and  $W_s$  is the probability of their capture in  $E_{ed}$ , it follows that the observable magnitude of the effect is

$$\Delta\rho/\rho \approx -\frac{\Delta n}{n} = -\frac{\Delta R}{R} = \frac{R_{sat} - R}{R},$$

where  $R$  and  $R_{sat}$  can be easily calculated from Eq. (6), and  $R_{sat}$  corresponds to  $\alpha \rightarrow \infty$ . Obviously, the measured  $\tau_1^*$  must

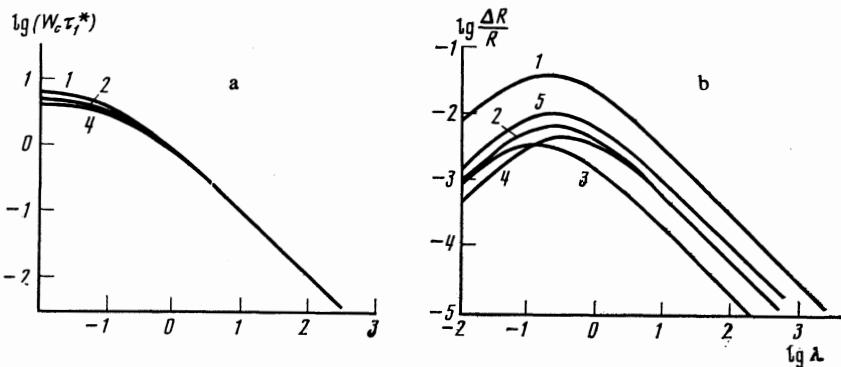


FIG. 8. Theoretical curves for  $\tau_1^*$  (a) and  $\Delta R / R$  (b), calculated from formulas (6) 1— $N = 1, \alpha = 10^{-5}$ ; 2— $N = 8, \alpha = 10^{-5}$ ; 3— $N = 8, \alpha = \lambda$ , 4— $N = 8, \alpha = 0.1$ ; 5— $N = 15, \alpha = 10^{-5}$  (with account taken of  $H_{ee}$ ).

correspond in first-order approximation to the average lifetime (7).

We have so far not taken into account the possibility of exchange interaction  $H_{ee}$  between the electrons in  $E_{ed}$  and the DDB. If  $H_{ee}$  is larger than the distance between the EPR lines of the BDB and of the electrons in  $E_{ed}$ ,  $H_{ee} \gg \Delta g g^{-1} H_0$ , which is quite probable, then the projection of the spin of the electron in  $E_{ed}$  on the average spin of the chain will not oscillate at the difference frequency  $|g_c - g_{DDB}|/\gamma H_0$ . We can then choose the quantization axis for the average polarization of the chain  $\bar{p}_2$  the spin direction of the electron in  $E_{ed}$ , i.e., there is no need to integrate with respect to  $p_1$  in (5)–(7), and we can simply put  $p_1 = 1$ . Calculation shows that the form of the functions  $\Delta R / R(\alpha; \lambda; N)$  and  $\tau_1^*(\alpha; \lambda; N)$  is changed little thereby (see Fig. 8), but the magnitude of the effect increases by approximately 2.8 times.

It should be noted that at  $H_{ee} \gg H_0$  the magnetic resonance will correspond to precession of the total angular momentum of the chain as a whole. In the case of large  $H_{ee}$ , however, the SDR effect can be observed, since saturation of the EPR signal of the DDB should lead to heating up of the exchange reservoir, corresponding to a change of  $\bar{p}_2$ . (In this paper we do not consider the situation in which  $H_{ee}$  is so large that the indirect ferromagnetic interaction that arises between the DDB spins leads to a change in  $\bar{p}_2$  of the chain upon capture of an electron in  $E_{ed}$ . The calculation formula should in this case have a different form and the SDR should be larger.)

The calculated relations

$$\frac{\Delta R}{R} = \frac{R(\alpha + \alpha_{mw}) - R(\alpha)}{R(\alpha)}$$

as functions of the spin-flip probability in the microwave field  $\alpha_{mw}$  are shown in Fig. 4. It was assumed that

$$\bar{\alpha}_{mw} = W_f \text{ mw} / W_c = \gamma H_1^2 / W_c \cdot 8H_M,$$

where  $H_M$  is the amplitude of the modulation of the magnetic field at  $f_M \gg (1/\tau_1; 1/\tau_1^*)$ ,  $H_M \gg \Delta H$ , where  $\Delta H$  is the width of the EPR lines. It was found that the calculated relations are quite close in form to relations of the type

$$\frac{1/4 \gamma^2 H_1^2 \tau_{eff} \tau_2^*}{1 + 1/4 \gamma^2 H_1^2 \tau_{eff} \tau_2^*},$$

where  $\tau_2^* \approx (2\gamma H_M)^{-1}$ , which correspond to the usual curves of the saturation of the EPR spectrum with  $\tau_1$  replaced by  $\tau_{eff}$ , the latter being a certain combination of  $\tau_1$ ,  $W_D$ , and  $W_c$  (in first-order approximation we have  $\tau_{eff}^{-1}$

$\approx (\tau_1^*)^{-1} + (\tau_1)^{-1}$ ). It is seen that the agreement with experiment is good.

Figure 8 shows the calculated dependences of the SDR  $\Delta R / R$  (corresponding to  $H_1 \rightarrow \infty$ ) and  $\tau_1^*$  for certain values of the parameters.  $\Delta R / R$  decreases approximately like  $N^{-1}$ . The quantity  $\tau_1^*$ , as expected, depends little on  $N$ , and  $\tau_1$  is determined mainly by the parameters  $W_D$  and  $W_c$ .

#### 4.2 Dependences of $\tau_1^*$ , $\tau_1$ , and $\chi'$ on the illumination level

We discuss now the dependences of  $\tau_1^*$  and  $\tau_1$  on  $\rho$ , plotted in Fig. 3(a). The simplest way of explaining the dependence of  $\tau_1$  on the density of the free carriers is to take into account the exchange interaction of the DDB with the free electrons and holes. A decrease of  $\tau_1$  upon illumination was observed in Ref. 21 for paramagnetic  $Fe^0$  centers in Si. Indeed, in the presence of photoelectrons, the relaxation of the DDB spins described by the expressions

$$\begin{aligned} \beta_{DDB} &= -nU(\beta_{DDB} - \beta_e) - \frac{\beta_{DDB} - 1/T}{\tau_1^0}, \\ \beta_e &= -N_{DDB}U(\beta_e - \beta_{DDB}) - \frac{\beta_e - 1/T}{\tau_{1e}^0} - \frac{\beta_e}{\tau_e}, \end{aligned} \quad (8)$$

where  $\beta_{DDB}$  and  $\beta_e$  are the reciprocal spin temperatures of the DDB and of the electrons,  $\tau_1^0$  and  $\tau_{1e}^0$  are the times of the spin-lattice relaxation of the DDB and of the electrons,  $\tau_e$  is the electron lifetime,  $U$  is the exchange probability,  $U = 2\langle V_e \rangle \sigma$ , where  $V_e$  is the thermal velocity of the electrons and  $\sigma$  is the cross section for exchange interaction of the electron with the DDB.

Similar equations were solved in Ref. 21:

$$\tau_1 \approx \frac{nU[(\tau_{1e}^0)^{-1} + \tau_e^{-1}]}{N_{DDB}U + \tau_e^{-1} + (\tau_{1e}^0)^{-1}}, \quad (9)$$

and

$$\begin{aligned} \beta_{DDB} &\approx \frac{\chi_0 DDB}{\chi_{DDB}} \\ &\approx \frac{nU(\tau_{1e}^0)^{-1} T^{-1} + (\tau_1^0)^{-1} (N_{DDB}U - (\tau_{1e}^0)^{-1} + \tau_e^{-1}) T^{-1}}{nU[(\tau_{1e}^0)^{-1} + \tau_e^{-1}] + (\tau_1^0)(N_{DDB}U + (\tau_{1e}^0)^{-1} + \tau_e^{-1})}. \end{aligned} \quad (10)$$

According to Hall-effect data, the mobility of the free carriers in our samples is  $\mu \approx 600 \text{ cm}^2 \cdot \text{s}^{-1} \cdot \text{V}^{-1}$ , so that knowing the resistivity we can estimate the carrier density. Figure 3 shows the calculated plots for  $\tau_1$  and  $\chi_{DDB}$ , with the values of  $U$ ,  $\tau_{1e}^0$ , and  $\tau_e$  fitted by minimizing the mean squared deviation. The curves correspond to the values  $U \approx 2 \times 10^{-6}$  and

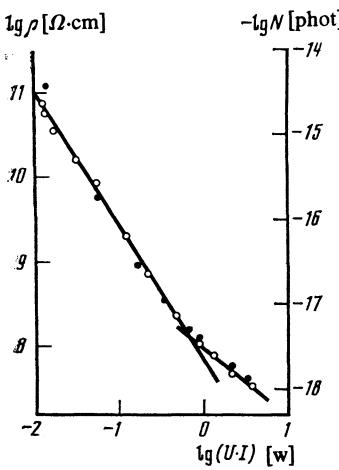


FIG. 9. Dependence of the resistance of the sample (O) and of the number of photons absorbed by the sample (●) on the lamp power at  $T = 1.4$  K.

$\tau_e^0 \approx \tau_e \approx 3 \times 10^{-11}$  sec. It can be seen that the agreement is not very good. In addition, direct measurements<sup>22</sup> yield at helium temperatures  $\tau_{1e}^0 \gtrsim 10^{-5}$  sec.

As for the quantity  $\tau_e$  it can be formally estimated in the following manner: Fig. 9 shows the dependence of the sample resistance on the power absorbed by the illuminating lamp. The same figure shows the number of photons absorbed by the sample, divided by the sample volume. The calculation was based on the formula

$$G = \int_{0.6 \text{ eV}}^{1.1 \text{ eV}} kN_{ph}(E)A(E)dE,$$

where  $k$  is a geometric factor,  $N_{ph}(E)$  is the spectral density of the radiated photons, which is close to  $N_{ph}(E)$  of a black body, and  $A(E)$  is the absorption coefficient of the sample. It was assumed that  $A(1.1 \text{ eV}) = 1$ , and the  $A(E)$  spectral dependence coincides with the spectral dependence of the photoconductivity measured in Ref. 17 (where samples with the same dislocation density and with approximately the same dimensions were used). From a comparison of the curves in Fig. 9 it follows that the lifetime of the carriers is  $\tau_e \gtrsim 4 \times 10^{-10}$  sec. From such a rough estimate it is quite clear that the real  $\tau_e > 3 \times 10^{-11}$  sec. Thus, the DDB interaction with the free carriers cannot explain the experiment.

The disparity can be resolved by recognizing that the carrier density in the sample is inhomogeneous because of the presence of band bending near the dislocations, due to the deformation potential of the dislocations. In this case the density near the dislocations can be many times larger than the density of the dislocations that determine the conductivity. Indeed, the dc conductivity is determined by the free carriers with energies above the percolation threshold. If the electron temperature is  $\approx 10$  K and the bottom of the conduction band near the dislocations is 10 meV lower than the percolation level, the local density is higher by five orders of magnitude than would follow from the conductivity. In addition, it must be recognized that the electrons and the holes are excited by the light in a substantially superheated state and then relax rapidly in energy with emission first of optical and then of acoustic phonons. In this case rapid thermaliza-

tion of their spins should also take place. It is therefore necessary to use a certain  $\tau_{1e}^{\text{eff}} \ll \tau_{1e}$ . Thus, the dependence of  $\tau_1$  on  $\rho$  can be understood, at least qualitatively, by taking into account the presence near the DDB, due to the deformation potential.

As follows from Fig. 3a, the parameter  $\tau_1^*$ , which is determined by the ratio of  $W_D$  and  $W_c$  [see Fig. 8(b)] also depends strongly on the illumination level. It can be assumed that the activation of the carriers from the levels  $E_{ed}$  and  $E_{hd}$  is not thermal means but is due also, e.g., to Auger processes.

#### 4.3 Comparison of experimental data on SDR with the proposed model

Figure 6 shows the experimental dependence of  $\Delta\rho/\rho$  on  $\tau_1^*$  at 1.4 K, and the calculated relation obtained from (6) to (7) at  $N = 8$  and  $W_c = 63 \text{ sec}^{-1}$ . In the presence of exchange interaction between the DDB and the electrons in  $E_{ed}$  and  $H_{ee}$ , calculation yields a similar dependence at  $N = 20$ . The value of  $W_D$  was obtained from  $\tau_1^*$ , while  $W_f$  was estimated by extrapolating the EPR data [Fig. 3(a)]. It can be seen that the agreement with experiment is good.

Figure 5(b) shows an attempt to compare the temperature dependence of  $\Delta\rho/\rho$  with the calculation. Unfortunately, we do not know the exact dependences of  $W_c$  and  $W_D$  on  $T$ , and experimental data on  $\tau_1(T)$  are available only in the region  $T > 25$  K (Ref. 2) [curve 1 of Fig. 5(a)]. Curve 1 for  $\tau_1$  in Fig. 5(a) was drawn for the region  $6 \text{ K} < T < 25 \text{ K}$  by using a highly approximate extrapolation formula proposed in Ref. 2. The dashed curve 1 of Fig. 5(b) was calculated from these data for  $\tau_1$  under the assumption that  $W_c = \text{const} = 63 \text{ sec}^{-1}$ , i.e., does not depend on the temperature. The agreement with experiment is in this case unsatisfactory. It must therefore be assumed that  $W_c$  depends on the temperature, which is perfectly reasonable, since an energy barrier can exist between  $E_2$  and  $E_{ed}$  (Fig. 7). Curve 1 of Fig. 5(b) and the calculated curve for  $\tau_1^*$  on Fig. 5(a), which agree well with experiment, and were obtained under the assumption that

$$\begin{aligned} W_c [\text{sec}^{-1}] &= 63 + 1.6 \cdot 10^5 \exp(-E^*/k_B T), \\ W_D [\text{sec}^{-1}] &= 25 + 1.9 \cdot 10^5 \exp(-E^*/k_B T), \end{aligned} \quad (11)$$

where  $E^* = 10 \text{ meV}$ ;  $N = 20$  (the  $H_{ee}$  exchange is present), and the values in the region  $T < 27$  K correspond to curve 2 on Fig. 5(a), i.e., the extrapolation formula of Ref. 2 underestimates somewhat the values in this temperature region.

Thus, the model proposed above can explain in principle all the experimental results both qualitatively and quantitatively.

We discuss now the requirements imposed by this model. We note first that for the model to be valid the spin chains, which are separate sections of the dislocations with DDB, should be sufficiently isolated from one another, so that the probability of inversion of the projection of the total spin of the chain on account of spin interactions, primarily dipole-dipole interactions, with the neighboring chains must not exceed the experimental values of  $W_f$ , i.e.,  $W_{da} \ll W_f$ . The minimum  $W_f$  observable in experiment at  $T = 1.4$  K

and under weak illumination corresponds to  $W_f = 10-20 \text{ sec}^{-1}$ .

We can roughly estimate the distance between the spin chains, which follows from the requirement  $W_{dd} \ll W_f$ . Generally speaking, the distance between the DDB in a dislocation core depends on the type of dislocation. For  $60^\circ$  dislocations this value is  $a^* \approx 3.8 \text{ \AA}$ . However, as shown in Ref. 2, at  $T < 45 \text{ K}$  the effective number of paramagnetic DDB decreases, and at  $T < 20 \text{ K}$  their number is 2–3 times smaller. It was proposed in Ref. 2 that this is due to the instability of the chains to variation of the period, which leads to a pairing of two out of three neighboring spins into a singlet state on account of the increase of the exchange interaction between them. As a result, the distance between the paramagnetic DDB at  $T < 20 \text{ K}$  can become of the order of  $3a^* \sim 10 \text{ \AA}$ . However, even when account is taken of this fact, the dipole-dipole interactions between them should give a EPR line width of the order of  $H_{dd} \approx \mu_B/(3a^*)^3 \approx 10 \text{ Oe}$ . Since the observed EPR line width is of the order of  $0.4-1 \text{ Oe}$  (Ref. 18), it must be assumed that an exchange interaction exists between the paramagnetic DDB and leads to a narrowing of the lines.<sup>23,24</sup> We then have

$$\Delta H = H_{dd}(H_{dd}/H_e),$$

where  $H_e$  is the exchange field. Whence  $H_e(T < 20 \text{ K}) \approx 200 \text{ Oe}$  (at  $T \gtrsim 50 \text{ K}$  the estimates of  $H_e$  are even larger). Thus, this is a lowerbound estimate of  $H_e$ . Let now the distance between the individual DB chains be of the order of  $r_0$ . We then have

$$W_{dd} [\text{sec}^{-1}] \approx \gamma (\mu_B/r_0)^2 / H_e \lesssim 15,$$

whence  $r_0 \lesssim 70 \text{ \AA} \approx 17a^*$ . Thus, the dislocation core should be as follows: there exist DDB chains, separated by sections of dislocations without DDB, of length  $(10-20)a^*$ . We note that if the real  $H_e$  is larger, then the sections without the DDB can be accordingly shorter. What is the average length of the DDB chains? From a comparison with experiment we obtain  $N_{\text{eff}} \approx 7-8$  in the absence of  $H_{ee}$  or  $N_{\text{eff}} \approx 20$  in the presence of exchange interaction  $H_{ee}$  between the DDB and the electrons in  $E_{ed}$ . If the lengths of the chains are described by a Gaussian distribution with parameters  $N$  and

$$X(N) = (1/\sqrt{2\pi}\kappa N) \exp \left[ -\frac{[(N-\bar{N})/\kappa\bar{N}]^2}{2} \right],$$

we have, assuming that  $\Delta\rho/\rho \propto 1/N$ ,

$$N_{\text{eff}}^{-1} \approx \int_1^\infty X(N) \frac{dN}{N},$$

from which we can obtain the dependence of  $\bar{N}$  on  $\kappa$ . As  $\kappa \rightarrow 0$  we have, obviously,  $\bar{N} = N_{\text{eff}}$ . At  $\kappa = 0.7-1.5$  we have  $\bar{N} \approx 2N_{\text{eff}}$ . Thus, the average length of the DDB chains is  $(14-40)a^*$ , depending on the presence of the exchange  $H_{ee}$ . It is precisely for this reason that the average distance between the DDB along the dislocations, calculated from the dislocation density  $N_D$  and from the DDB density, usually amounts to  $\bar{a} = N_D/N_{\text{DDB}} \approx 5-7 \text{ \AA}$  in place of the expected  $3.5-4 \text{ \AA}$ .

Let us discuss the possible cause of the onset of sufficiently extended sections without DDB. As already noted, when the samples are annealed at  $T \gtrsim 700 \text{ }^\circ\text{C}$ , the EPR signal

of the DDB vanishes. This was investigated in detail in Ref. 15, where it was suggested that the most probable mechanism is the reconstruction of the dislocation cores in such a way that the DDB are pairwise closed to form covalent bonds. The energy gain due to the formation of covalent bonds compensates for the increase in energy on account of the lattice deformation.<sup>25</sup> The energy difference is apparently large enough and exceeds  $k_B T$  when  $T$  is lower than the melting temperature, therefore the reconstruction is irreversible, in contrast to a transition that occurs in DDB chains at  $T \lesssim 50 \text{ K}$ . The existence of nonreconstructed chains is due to the high activation energy for the reconstruction process, and is a nonequilibrium situation.

The substantial differences between this model of DDB annealing and the model with diffusion of impurities to the dislocations with formation of DDB + impurity-atom bonds consists in the fact that in the impurity mechanism the DDB should vanish one by one at arbitrary points of the dislocation. In the case of the model with reconstruction, by virtue of the collective character of the process, the DDB should close immediately on sufficiently long sections of the dislocations, bounded apparently by certain pinning points, e.g., jogs or impurity atoms.

It should be noted that favoring the reconstruction of the dislocations upon annealing are, as is now clear, certain results, of Ref. 23. In Ref. 23 they investigated the ratio of the integral intensities of the EPR spectra of the DDB and of the neutral phosphorus atoms at  $T = 1.3 \text{ K}$ . When the dislocations are introduced, the intensity of the EPR signal from the phosphorus decreases because of the capture of electrons by the DDB (into the  $E_2$  band). The ratio of the number of captured electrons  $N_e$  to the number of the DDB,  $N_{\text{DDB}}$ , namely  $f = N_e/N_{\text{DDB}}$ , was always less than 0.2, this being due to the Coulomb interaction of the electrons captured by the dislocations. Upon annealing of the samples it was found that  $N_e$  decreases in proportion to the decrease of  $N_{\text{DDB}}$ , i.e.,  $f \approx \text{const}$ . This can be explained only by assuming that the DDB vanishes at once over sufficiently long sections of dislocations ( $> 5a^*$ ), and on the remaining sections the distance between the DDB remains the same as before and their length is also larger than  $5a^*$ . In the opposite case  $N_e$  would start to decrease only after the vanishing of 80% of the DDB.

## 5. CONCLUSION

Thus, the experimental results can be qualitatively and quantitatively understood on the basis of the following model: the dislocation core contains spin chains of DDB, whose average length is of the order of 15–40 spins. The chains are separated by dislocation sections without free spins, and the maximum length of these sections needed for the model to be valid is 10–20 lattice constants. The recombination of the free carriers proceeds as follows: the electrons and holes are captured (with arbitrary spin directions) near the dislocation cores into shallow states which can be due to the deformation potential that is present. They are next either activated back into bands, or captured on the dangling bands (DDB) in the singlet state, followed by recombination. The spin-dependent is only the capture of the electrons (or holes) from a

shallow state on the DDB chain. The capture probability depends here on the polarization of the given chain along the electron-spin direction.

At magnetic resonance, the chain polarization begins to vary with time, and if these changes occur within times much shorter than the electron lifetime in the shallow state, the recombination probability of those electrons that have formed triplet configurations with DDB increases. The SDR is then independent in first-order approximation of the external magnetic field.

An analysis of the dependence of the time of the spin-lattice relaxation of the DDB on the illumination level also shows the need for taking into account the band bending due to the deformation potential of the dislocations.

In the calculations of the value of the SDR we have neglected the DDB polarization due to the external magnetic field  $H_0$ , allowance for which should apparently add to the calculated value an increment of the order of

$$(\mu_B H_0)^2/k_B^2 T_e (T_{\text{DDB}} + T_N),$$

where  $T_e$  and  $T_{\text{DDB}}$  are the spin temperatures of the electrons and of the DDB, and  $T_N$  is the Neel temperature of the DDB. In addition, we did not take into account the influence of the various exchange interactions between the DDB in the chain, capable of changing the distribution of the probabilities  $W(p_2)$  of observing a given polarization  $p_2$  of a finite chain. Allowance for the last circumstance can change the estimates for the chain length.

<sup>1</sup>V. V. Kveder and Yu. A. Osip'yan, Zh. Eksp. Teor. Fiz. **80**, 1206 (1981) [Sov. Phys. JETP **53**, 618 (1981)].

- <sup>2</sup>V. A. Grazhulis, XV. V. Kveder, and Yu. A. Osip'yan, Phys. State. Sol. (b). **103**, 519 (1981).
- <sup>3</sup>V. V. Kveder, Yu. A. Osip'yan, W. Schröter, and G. Zoth, ibid., to be published.
- <sup>4</sup>D. Lepine, V. A. Grazhulis, and D. Kaplan, Proc. 13-th Conf. Phys. of Semicond. Rome, 1976.
- <sup>5</sup>D. Lepine, Phys. Rev. **B6**, 436 (1972).
- <sup>6</sup>V. A. Grazhulis, V. V. Kveder, and Yu. A. Osip'yan, Pis'ma Zh. Eksp. Teor. Fiz. **21**, 708 (1975) [JETP Lett. **21**, 335 (1975)].
- <sup>7</sup>T. Wosinski and T. Figiel'ski, Phys. Stat. Sol. (b), **71**, K73 (1975).
- <sup>8</sup>T. Wosinski and T. Figiel'ski, ibid., **83**, 93 (1977).
- <sup>9</sup>R. M. White and J. F. Gouyet, Phys. Rev. **B16**, 3596 (1977).
- <sup>10</sup>J. F. Gouyet, J. de Phys. **40**, 107 (1979).
- <sup>11</sup>P. Kaplan, I. Solomon, and N. E. Mott, J. de Phys. Lett. **39**, L51 (1978).
- <sup>12</sup>L. S. Mima, V. I. Strikha, O. V. Tretyak, Fiz. Tekh. Poluprovodn. **14**, 2242 (1980) [Sov. Phys. Semicond. **14**, 1328 (1980)].
- <sup>13</sup>I. Solomon, D. Iegelsen, and J. C. Knights, Sol. St. Commun. **22**, 505 (1977).
- <sup>14</sup>M. H. Brodsky and R. S. Title, Phys. Rev. Lett. **23**, 581 (1969).
- <sup>15</sup>M. N. Zolotukhin, V. V. Kveder, and Yu. A. Osip'yan, Zh. Eksp. Teor. Fiz. **81**, 299 (1981) [Sov. Phys. JETP **54**, 160 (1981)].
- <sup>16</sup>V. A. Grazhulis and Yu. A. Osip'yan, ibid. **58**, 1259 (1970) [**31**, 677 (1970)].
- <sup>17</sup>V. A. Grazhulis, V. V. Kveder, and V. Yu. Muhina, Phys. Stat. Sol. (a) **43**, 407 (1977).
- <sup>18</sup>S. V. Broude, V. A. Grazhulis, V. V. Kveder, and Yu. A. Osip'yan, Zh. Eksp. Teor. Fiz. **66**, 1469 (1974) [Sov. Phys. JETP **39**, 721 (1975)].
- <sup>19</sup>V. A. Grazhulis, V. V. Kveder, and Yu. A. Osip'yan. Proc. 20th Congress Ampere, Tallinn, 1978.
- <sup>20</sup>V. L. Bonch-Bruevich and V. B. Glasko, Fiz. Tverd. Tela (Leningrad) **3**, 36 (1961) [Sov. Phys. Solid State **3**, 26 (1961)].
- <sup>21</sup>M. F. Deigen, V. Ya. Bratus', B. E. Vugmeister, and I. M. Zaritskii, Zh. Eksp. Teor. Fiz. **69**, 2110 (1975) [Sov. Phys. JETP **42**, 1073 (1975)].
- <sup>22</sup>R. J. Elliot, Phys. Rev. **96**, 266 (1954).
- <sup>23</sup>V. A. Grazhulis and Yu. A. Osip'yan, Zh. Eksp. Teor. Fiz. **60**, 1150 (1971) [Sov. Phys. JETP **33**, 623 (1971)].
- <sup>24</sup>S. A. Al'tshuler and V. M. Kozyrev, Electronnyi paramagnitnyi rezonans (Electron Paramagnetic Resonance), Nauka, 1972.
- <sup>25</sup>S. Marklund, Phys. Stat. Sol. (b) **92**, 83 (1979).

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