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PHOTO-ELECTRICAL EPR OF THE EXCITED TRIPLET STATES OF STRUCTURAL DEFECTS IN IRRADIATED SILICON

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Abstract

Upon illumination some structural defects in irradiated silicon can be excited into the metastable triplet S=1 states. This paper reports on the properties of their electron paramagnetic resonance (EPR) spectra detected by means of DC- and microwave-photoconductivity changes under magnetic resonance conditions. It has been concluded that, for microwave photoconductivity, the intensity of spectral lines depends quadratically on the square root of the microwave power in the cavity. This is in contrast to the usual EPR, for which the dependence is known to be linear. Also, the angular dependence of line intensities for the structural defects in their excited triplet states was investigated and spin-Hamiltonian parameters of the Si-PT1 and Si-PT4 spectra have been determined.

The spin-dependent recombination (SDR) phenomenon was first reported by Lepine [1]. It is based on a variation of photoexcited-carriers recombination rate upon the spin state of the recombination center and can be of interest as a nonstandard detection technique of electron paramagnetic resonance (EPR). Such a technique usually requires electrical contacts to the sample as the resonant variation of the photoconductivity is being measured. In addition a similar, but contact-free, technique of the SDR-spectra detection has also been proposed [2-4]. In a contact-free experimental scheme variations of the cavity-Q-factor value reflect the resonant changes in losses of the electric microwave field component due to the absorption by photoexcited free carriers. When applicable, this method appears to be more sensitive than conventional EPR by a few orders of magnitude. In the past it has served to detect several new spectra of the radiation defects in excited triplet states Si-PT1 [2], Si-PT3 [2], Si-PT4 [3], and Si-PT5 [4].

In the present paper the main properties of the EPR detection method based on the microwave-photoconductivity measurements are investigated and compared with DC-photoconductivity based detection. The method is subsequently applied for determination of spin-Hamiltonian parameters for the Si-PT1 and Si-PT4 spectra.

The experiments were carried out on samples prepared from high-resistivity (300 Ω·cm) float-zoned n-type phosphorus-doped silicon exposed to irradiation by 1–MeV

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electrons to the dose $\approx 10^{16} - 10^{18}$ cm^{-2}. EPR and SDR measurements were performed at a temperature of 10–12 K on an X-band superheterodyne spectrometer equipped with a cylindrical TE_{011} cavity and magnetic-field modulation at 12.3 Hz. In the experiment the sample was displaced by about a quarter of the radius from the axis of the cavity in order to have both electric and magnetic components of microwave field. It was illuminated via a quartz rod by a high-pressure 200-W xenon lamp. The DC-photoconductivity measurements were performed in a 2-contact configuration [1].

The investigated spectra are depicted in Fig. 1. At low microwave power levels of $\approx 10\mu$W the Si-PT1 spectrum has been detected in samples exposed to higher ($\sim 10^{18}$ cm^{-2}) irradiation doses. Under these experimental conditions the spectrum could, for the first time, be observed in conventional EPR, both in absorption and dispersion. As can be seen from Fig. 2 the phases of high- and low-field lines of the spectrum are opposite. The low- and high-field lines correspond to absorption and to emission of the microwave power, respectively. At higher microwave power both lines have the same phase and are detectable only in absorption mode.

In Fig. 3 the intensity of the Si-PT1 spectrum is plotted against the square root of the incident microwave power P. One can notice that the intensities of both low- (○) and high- (□) field lines depend quadratically on $\sqrt{P}$, whereas for the contact technique (+) the dependence is linear. This behaviour supports the assumption that for the contact-free scheme the observed signal is due to absorption of the electric field component (E) by photoexcited free carriers. The losses of microwave power are

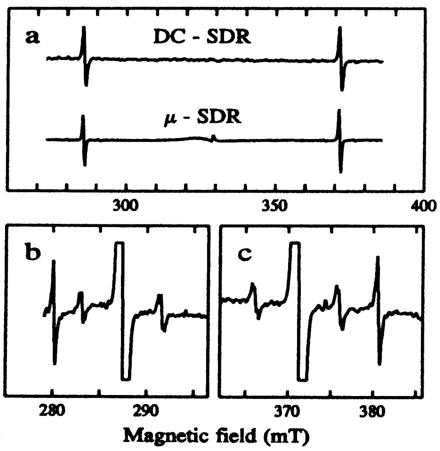

Fig. 1. EPR spectra in electron-irradiated silicon. **a**: spectrum Si-PT1, detected by DC- and microwave-photoconductivity variations; **b** and **c**: enlarged parts of spectrum Si-PT1 with ^{29}Si hyperfine satellites. Sharp lines at 280 and 381 mT belong to the spectrum Si-PT4.

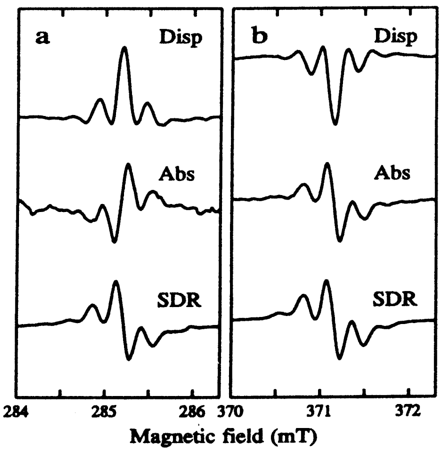

Fig. 2. Low- (**a**) and high- (**b**) field lines of Si-PT1 detected under conditions of the conventional EPR, in dispersion and absorption modes, and by microwave photoconductivity changes. Gain for EPR signals is 10^3 higher than for SDR. B$\|$<111>, T=10.2 K, ν=9.213648 GHz.

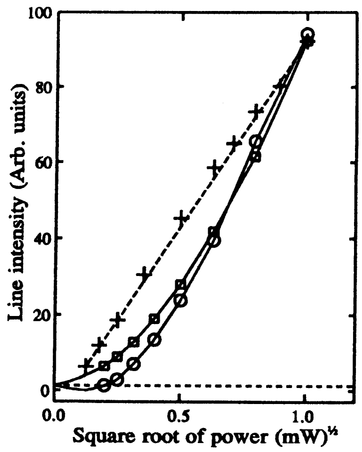

Fig. 3. Si-PT1 spectrum line intensity dependence on the microwave power. o -low-field, □ -high-field line, detected by microwave-photoconductivity variations. + -high-field line, detected by DC-photoconductivity variations.

then proportional to the product of the amplitude of this component and the concentration of free carriers. The variation of the latter is proportional to the number of EPR transitions which (in absence of saturation) is, in turn, proportional to the amplitude of the magnetic field component (H). Consequently, the SDR signal is proportional to $E \cdot H \sim P$. In case of DC-photoconductivity detection the electric component does not participate in the process and consequently the observed intensity is proportional to $H \sim \sqrt{P}$.

A characteristic feature of the EPR spectra for excited triplet states of several radiation defects (Si-PT1, PT3, PT4, PT5) is the strong angular dependence of their lines intensity. The angular dependence of the Si-PT1 SDR spectrum is shown in Fig. 4. As can be seen the experimental points could only be measured in a relatively small range of angles close to [111]. Assuming that the observed spectrum is associated with an $S = 1$ state and the two lines belong to two transitions $M_S : \pm 1 \leftrightarrow 0$, then the data can be very well fitted with a spin Hamiltonian containing Zeeman and fine-structure terms of trigonal symmetry along a <111> crystal axis, with following parameters: $g_{\|} = 2.007(6)$, $g_{\perp} = 2.002(5)$, and $D = \pm 1206.(8)$ MHz. The hyperfine splitting (see Fig. 1) arises from interaction with one ^{29}Si ($I = 1/2$, 4.7% abundance) and for $B \|$<111> the hyperfine-constant value $A = 28(5)$ MHz could be estimated.

Under similar assumptions as for Si-PT1, the Si-PT4 spectrum could be fitted with a spin Hamiltonian of monoclinic symmetry, with the following values of **g** and **D** tensors: $g_1 = 2.004(9)$, $g_2 = 2.011(5)$, $g_3 = 2.026(5)$, $\theta_g = 34.(2)^\circ$, $D_1 = \pm 983.(7)$ MHz, $D_2 = \mp 285.(5)$ MHz, $D_3 = \mp 698.(1)$ MHz, $\theta_D = 31.(0)^\circ$. The principal axes of g_2 and D_2 are parallel to the $[0\bar{1}1]$ direction; axes of g_1 and D_1 are not far from [111] and make angles θ_g and θ_D with [011], respectively.

The angle-dependent line intensity shown in Fig. 4(**b**) has been observed by microwave-photoconductivity measured SDR. The conventional EPR and DC-photoconductivity SDR have a similar intensity dependence. It can be associated with anisotropy of the transition probabilities R^+, R^o, and R^-, from spin states $|+1\rangle$, $|0\rangle$, and $|-1\rangle$, respectively, to the ground state of the defect[5]. If one assumes $R^+ = R^- = R \neq R^o$, the kinetic considerations [2] will give the following formula for the line intensities $I_\pm$ corresponding to transitions $|\pm 1\rangle \leftrightarrow |0\rangle$:

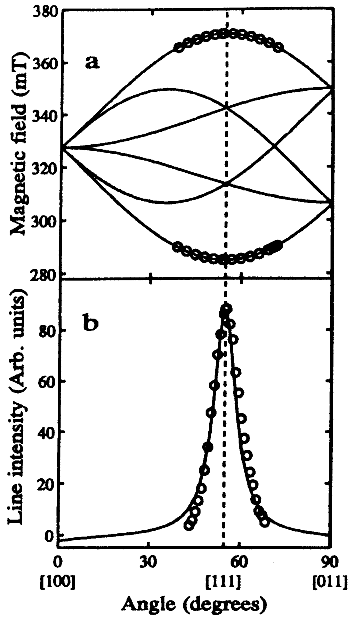

Fig. 4. Angular dependence of resonance field (**a**) and line intensity (**b**) of Si-PT1 spectrum. o - experiment; solid lines - computer fit.

$$I_{\pm} = \pm \frac{\Gamma(R - R^o)}{RR^o + W(2R + R^o)}, \qquad (1)$$

where Γ is the rate at which defects are excited into the triplet state under illumination and W is the spin-relaxation rate. The difference between R and R^o arises from spin-orbit interaction. This difference and the low spin-relaxation rate ($W \ll (2R+R^o)$) are responsible for a non-equilibrium population distribution between magnetic sublevels of the triplet center, which leads to phase inversion of EPR signals (see Fig. 2).

From direct calculations the angular dependence of R and R^o parameters can be obtained:

$$R = \rho \cos^2 \phi; \; R^o = \frac{1}{2} \rho \sin^2 \phi, \qquad (2)$$

where ϕ is the angle between magnetic field and <111> crystallographic axis. The experimental data can be fitted to formulae (1) and (2) with the parameter $W/\rho = 3 \cdot 10^{-3}$.

Concluding, it should be emphasized that independent measurements of both microwave and DC photoconductivity bring experimental evidence that excited triplet states of structural defects play an important role in the process of spin-dependent recombination of photoexcited carriers. The quadratic dependence of SDR-line intensity on power proves that absorption of microwave field electric component is responsible for the signals detected.

For two of such defects, Si-PT1 and Si-PT4, EPR and SDR spectra are studied in detail and spin-Hamiltonian parameters could be determined. The observed angular dependence of line intensities could be described by assuming the angular variation of relevant recombination rates.

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