

EPR OF PHOSPHORUS IN COMPENSATED n-TYPE Si SUBJECTED TO UNIAXIAL COMPRESSION

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The influence of uniaxial compression on the magnitude of the hyperfine splitting A in the EPR spectrum of phosphorus in n-type silicon was investigated at 1.3°K. This investigation was carried out on samples in which the phosphorus concentration was $N_D = (5-7) \cdot 10^{17} \text{ cm}^{-3}$ and whose degree of compensation was 60-99%. The dependence of the value of A on the uniaxial compression of these silicon crystals was identical with that for lightly doped silicon. This indicated that the compensation of heavily doped silicon resulted in the formation of localized states. The value of A decreased with increasing degree of compensation at zero applied pressure because of a correlation in the distribution of impurity atoms. It was established that the two causes of the fall in the value of A (uniaxial compression and compensation) were independent in the investigated range of uniaxial pressures (up to 30 kgf/mm²).

The magnitude of the hyperfine splitting A in the EPR spectra of shallow donors in silicon may be reduced in two ways. First, the value of A may be reduced by uniaxial compression along the [100] and [110] axes. This effect is due to the admixture of an excited doublet state to the ground singlet state of a donor impurity because of the compression-induced change in the populations of the conduction-band valleys [1]. Secondly, the strong compensation of heavily doped n-type silicon may alter the value of A because of the Stark effect [2]. It is not clear whether there is any relationship between these two types of the reduction in the value of A .

The purpose of our experimental investigation was to find whether such a relationship existed.

EXPERIMENTAL INVESTIGATION AND RESULTS

Our experiments were carried out on n-type silicon, doped with phosphorus ($N_D \sim 5 \cdot 10^{17} - 7 \cdot 10^{17} \text{ cm}^{-3}$) and compensated with boron ($K \sim 60-99\%$). The properties of the investigated samples and the hyperfine splitting at zero pressure, A_0 , are given in Table 1.

The EPR spectra were recorded by means of a spectrometer with direct amplification and high-frequency (100 kHz) modulation. These spectra were recorded at 1.3°K. The uniaxial compression was applied along the [100] crystallographic axis at right angles to the static magnetic field.

The values of A_0 were determined as a function of the degree of compensation, keeping the phosphorus concentration approximately constant. The results are presented in Table 1. It is evident that, in the absence of compensation, A_0 is 42 Oe.

TABLE 1

Sample No.	Phosphorus concentration, cm^{-3}	Degree of compensation K , %	ρ , $\Omega \cdot \text{cm}$	HFS splitting, Oe
1	$3.5 \cdot 10^{16}$	< 0.1	0.20	42
2	$5 \cdot 10^{17}$	< 0.1	0.03	42
3	$5 \cdot 10^{17}$	60	0.06	41
4	$7 \cdot 10^{17}$	95	0.35	37 ± 0.5
5	$7 \cdot 10^{17}$	99	0.45	37 ± 0.5

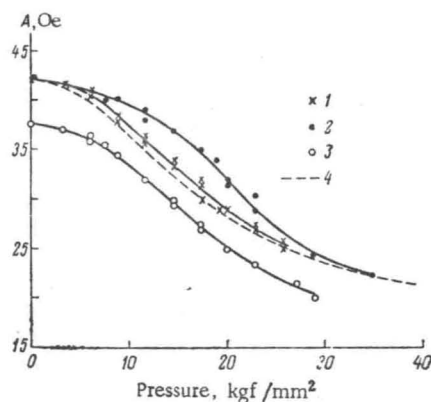


Fig. 1. Dependence of the hyperfine splitting A in the EPR spectra of n -type Si on the uniaxial compression along the $[100]$ axis. 1) Sample with $N_D = 3 \cdot 10^{16} \text{ cm}^{-3}$, $K < 0.1\%$; 2) sample with $N_D = 5 \cdot 10^{17} \text{ cm}^{-3}$, $K < 0.1\%$; 3) sample with $N_D = 7 \cdot 10^{17} \text{ cm}^{-3}$, $K = 99\%$; 4) theoretical dependence for $N_D = 1 \cdot 10^{16} \text{ cm}^{-3}$ [3].

When the compensation is increased, A_0 decreases to 37 Oe for $K = 99\%$.

The experimentally obtained dependence of the hyperfine splitting on the uniaxial compression is presented in Fig. 1 for silicon samples with a phosphorus concentration of $N_D = 7 \cdot 10^{17} \text{ cm}^{-3}$ and $K = 99\%$. This figure includes also the theoretical dependence (dashed curve) deduced in [3] for lightly doped silicon (phosphorus concentration $N_D = 1 \cdot 10^{16} \text{ cm}^{-3}$), as well as the experimental dependences [4] for silicon with phosphorus concentrations of $N_D = 3 \cdot 10^{16}$ and $5 \cdot 10^{17} \text{ cm}^{-3}$. Figure 2 shows the dependence of the ratio A/A_0 on the uniaxial compression (A_0 is the hyperfine splitting at zero pressure). It is evident from Fig. 2 that the dependence for our heavily doped sample is identical with the dependence for lightly doped uncompensated silicon.

DISCUSSION OF RESULTS

1. Penin, Zhurkin, and Volkov [2] suggested an explanation of the reduction in the hyperfine splitting A_0 in the EPR spectrum of phosphorus caused by strong compensation.

A detailed discussion of this point is given in [5], where it is shown that the electric fields of the charged donors and acceptors alter the positions of the energy levels of the donor electron. The $1s$ ground state, for which the probability of finding an electron at the site of an impurity nucleus $|\Psi(0)|^2$ is finite, acquires an admixture of the $2p$ excited state, for which $|\Psi(0)|^2 = 0$. This reduces the value of A because $A \propto |\Psi(0)|^2$. The splitting of the energy levels of the donor electron by the electric field of ionized impurity atoms (the Stark

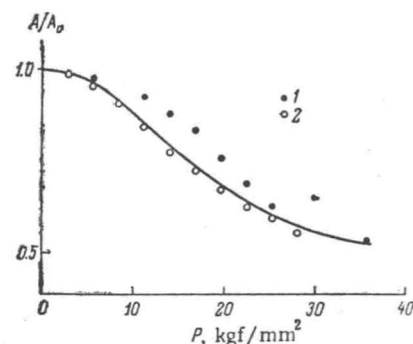


Fig. 2. Dependence of the relative hyperfine splitting A/A_0 on uniaxial compression along the $[100]$ axis (A_0 is the hyperfine splitting at zero pressure). 1) Sample with $N_D = 5 \cdot 10^{17} \text{ cm}^{-3}$, $K < 0.1\%$, $A_0 = 42$ Oe; 2) sample with $N_D = 7 \cdot 10^{17} \text{ cm}^{-3}$, $K = 99\%$, $A_0 = 37.5$ Oe; the continuous curve gives the pressure dependence A/A_0 for a sample with $N_D = 3 \cdot 10^{16} \text{ cm}^{-3}$, $K < 0.1\%$.

effect) depends strongly on the spatial correlation in the distribution of impurity atoms. The fields of the impurity centers are screened and since there are few free carriers, the screening is due to ionized impurities. Volkov [5] assumed that the potential of charged impurities is the screened Coulomb potential,

$$U(r) = \frac{e}{\epsilon r} \exp\left(-\frac{r}{l}\right),$$

where l is the screening radius and the donors are almost fully compensated by acceptors. Volkov [5] used these assumptions in the calculation of the reduction in A_0 , governed by the average value of the gradient of the electric field established by the impurity centers in the direct vicinity of a neutral donor:

$$\left| \frac{A_0^{\text{comp}} - A_0^{\text{isol}}}{A_0^{\text{isol}}} \right| = \frac{4\pi n}{l} \frac{|\langle 1s || r || 2p \rangle|^2}{(E_{1s} - E_{2p})^2},$$

where the superscripts "comp" and "isol" refer to compensated and isolated impurities, n is the impurity concentration ($n = 10^{18} \text{ cm}^{-3}$), and

$$E_{1s} - E_{2p} = 0.034 \text{ eV}.$$

The screening radius can be found by substituting the experimental value of A_0 into Eq. (1) and calculating the matrix element by means of hydrogen-like wave functions.

If the donor impurity concentration is $N_D = 7 \cdot 10^{17} \text{ cm}^{-3}$ and the degree of compensation is $K = 99\%$, the screening radius is $l = 10a^*$ (a^* is the effective Bohr radius in silicon). In this case, the average distance between impurity atoms is

$$r_{av} = 0.62 N_D^{-1/3} = 3a^*.$$

2. Keldysh and Tratas [6] showed that the compensation of an n-type semiconductor results in the pickup of the exchange bonds between donor electrons by the electric fields of charged impurity atoms. A relative increase in the amplitude of the hyperfine splitting lines was observed experimentally in [7, 8] for n-type compensated silicon. This indicated that localized states were formed.

An analysis of the dependence of the magnitude of the hyperfine splitting of the EPR lines of phosphorus in silicon ($N_D = 7 \cdot 10^{17} \text{ cm}^{-3}$, $K = 99\%$) on the uniaxial compression can give some information on the interaction of impurities in silicon.

Figure 2 shows the dependence of the relative splitting A/A_0 on the uniaxial compression applied to three samples with phosphorus concentrations of $N_D = 3 \cdot 10^{16}$, $5 \cdot 10^{17}$, and $7 \cdot 10^{17} \text{ cm}^{-3}$ ($K = 99\%$). It is evident from Fig. 2 that the experimental points fit the curve for the uncompensated silicon. This indicates that localized states are formed in the heavily doped and compensated silicon.

No theoretical expression is yet available for the influence of the electric fields of charged donors and acceptors on neutral impurities in a semiconductor subjected to uniaxial compression. However, the experimental results (Fig. 1) indicate that the curve for a compensated sample is identical with the curve for a lightly doped crystal, and is shifted from the latter by 4 Oe, which is equal to the difference between the values of the hyperfine splitting at zero pressure. Hence, we may conclude that, in the investigated range of uniaxial compression (up

to 30 kgf/mm^2), the two causes of the reduction in the hyperfine splitting (uniaxial compression and the Stark effect) are independent.

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LITERATURE CITED

1. D. K. Wilson and G. Feher, *Phys. Rev.*, **124**, 1068 (1961).
2. N. A. Penin, B. G. Zhurkin, and B. A. Volkov, *Proc. Ninth Intern. Conf. on Physics of Semiconductors*, Moscow, 1968, Vol. 2, Nauka, Leningrad (1968), p. 1122.
3. B. A. Volkov and N. B. Volkov, *Fiz. Tekh. Poluprov.*, **4**, 409 (1970) [*Sov. Phys.-Semicond.*, **4**, 345 (1970)].
4. V. B. Ginodman, P. S. Gladkov, B. G. Zhurkin, and N. A. Penin, *Fiz. Tekh. Poluprov.*, **4**, 325 (1970) [*Sov. Phys.-Semicond.*, **4**, 264 (1970)].
5. B. A. Volkov, *Brief Communications in Physics* [in Russian] (1970).
6. L. V. Keldysh and T. T. Tratas, *Fiz. Tverd. Tela*, **8**, 83 (1966) [*Sov. Phys.-Solid State*, **8**, 64 (1966)].
7. B. G. Zhurkin, N. A. Penin, and B. A. Volkov, *Fiz. Tverd. Tela*, **6**, 2558 (1964) [*Sov. Phys.-Solid State*, **6**, 2040 (1965)].
8. B. G. Zhurkin and N. A. Penin, *Fiz. Tverd. Tela*, **7**, 3204 (1965) [*Sov. Phys.-Solid State*, **7**, 2592 (1966)].