Impurity polarizability in silicon due to the magnetic degeneracy of donor states in a finite magnetic field

S. M. Dikman and D. I. Sidel'nikov
All-Union Scientific Research Institute for Current Sources

(Submitted 15 May 1991)
Pis'ma Zh. Eksp. Teor. Fiz. **53**, No. 12, 600–603 (25 June 1991)

It is shown theoretically that the crossing of the energy levels $E_i(H)$ of shallow donor states of different symmetries due to the anisotropy of the effective mass makes it possible to experimentally observe an anomalously high impurity polarization that is independent of the electric field.

1. If a field $\vec{H}$ is directed along one of the principal axes of a crystal, calculations show that level crossings (points of magnetic degeneracy) occur in silicon even in the lowest part of the spectrum. In these cases the diagonal matrix elements of the dipole moment are nonzero, and in the presence of an electric field the true crossing is transformed into an anticrossing. The gap between the split levels is proportional to the field $\vec{E}$. This effect in a nonhydrogen-like spectrum is, in a certain sense, even more accidental than the "accidental" degeneracy and the linear Stark effect for the hydrogen atom, since in the former case it is not related to any conservation law.

In this article we present the results of a calculation of the eight lowest levels, for just those electrons for which the principal axis of the effective mass is oriented along the magnetic field. Each of the levels is thus twofold degenerate. Depending on the type of impurity, this intervalley degeneracy is lifted if the field of the neutral cell is taken into account, but the splitting, as is well known,[1-3] is appreciable only for the ground state. Experiments[4] show a considerably smaller splitting than, for instance, the calculations in Ref. 2, a result that is, in our view, a consequence of an unfortunate choice made by those investigators[2] for the trial wave functions. Because of the axial symmetry, one can retain the same classification of the levels as in the problem of the hydrogen atom in a magnetic field[5,6] or in the problem of a donor in a semiconductor without a field.[1,7]

2. We used a variational method for the calculations. The dimensionless Schrödinger equation is written in the standard form[2,6] (the anisotropy parameter for silicon is $m_\perp/m_z = 0.208$), but the trial wave functions that we used have a different form. The recipe for the choice, following the ideas of Ref. 6, leads to the following form:

$$\Psi_i = R_i(\rho, z, \varphi)\exp[-\Phi_i(\rho, z, \varphi)]; \quad i = 1s,\ 2s,\ 2p_{\pm1},\ 2p_0,\ 3p_0,\ 3d_{-1},\ 3d_{-2}. \tag{1}$$

$$R_{1s} = 1,\ \ R_{2s} = Q_{2s},\ \ R_{2p_{\pm1}} = \rho e^{\pm i\varphi},$$

$$R_{2p_0} = z,\ \ R_{3p_0} = zQ_{3p_0},\ \ R_{3d_{-1}} = z\rho e^{-i\varphi},$$

$$R_{3d_{-2}} = \rho^2 e^{-2i\varphi}, \quad Q_1 = 1 - c_i\sqrt{m_i^2 + \sqrt{z^2 + d_i^2\rho^2} + s_i^2(\rho^2 + t_i^2 z^2)}\,,$$

$$\Phi_i = \sqrt{a_i^2(\rho^2 + b_i^2 z^2) + \sqrt{1 + H^2}(u_i\rho^2 + w_i z^2)\sqrt{z^2 + v_i^2\rho^2} + \frac{H^2}{16}\rho^4},$$

where a_i, b_i,... are variational parameters and H is the dimensionless magnetic field. The individual dimensionless quantities correspond to the actual values

$$\frac{m_\perp e^4}{2\hbar^2\epsilon^2} \cong 18.9\ \text{MeV}, \quad \frac{\hbar^2\epsilon}{m_\perp e^2} \cong 32.6A^\circ, \quad \frac{e^3 m_\perp^2 c}{\hbar^3\epsilon^2} \cong 620\ \text{kOe}\ .$$

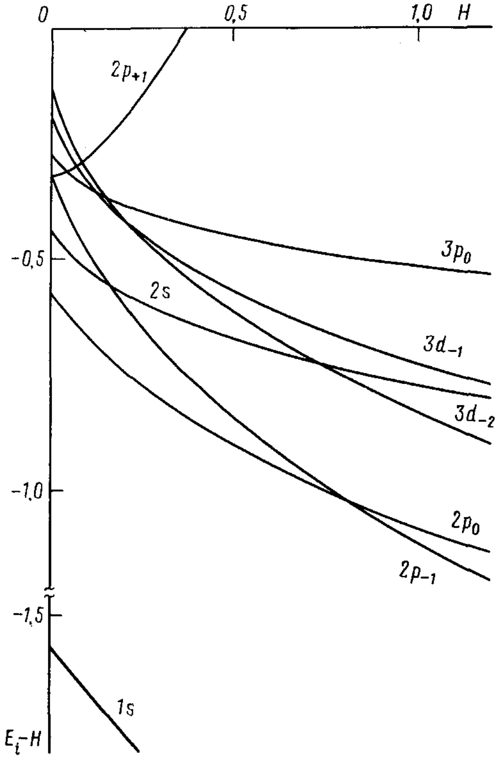

FIG. 1.

TABLE I.

$1s$; 1,567	$2p_{+1}$; 0,321	$2s$; 0,444	$3p_0$; 0,275	$2p_0$; 0,576	$3d_{-1}$
$3d_{-2}$; 0,132	0,085; 0,293	0,74;* 0,726	0,15;* 0,366	4,73; 1,651	0,21;* 0,422
$2p_{-1}$; 0.321		0.16;* 0,557		0.82;* 0,204	
$3d_{-1}$; 0.194	0,071; 0,301	1.59; 0,851	0,12;* 0,353		
$3p_0$; 0.275	0,045; 0,312				

The functions Ψ_{1s} and Ψ_{2s} are mutually orthogonal, as are Ψ_{2p0} and Ψ_{3p0}. A search was made for the optimal two-dimensional orthogonal basis for this pair of states by the method of Galerkin. Different indirect and direct tests showed that functions (1) with parameters determined by a solution of the spectral problem can be used for calculation of the matrix elements of the multipole moments.

3. The results of the calculations for the ionization energies are shown graphically in Fig. 1. The level crossings are listed in Table I (the first number is H and the second is H–E_i in dimensionless units). The binding energy in zero field is indicated next to the spectral index. The crossings that are due to the anisotropy of the effective mass are indicated by the asterisks (*).

Let us consider the $(2s, 2p_{-1})$ crossing. In a weak electric field perpendicular to $\vec{H}$ we find near the crossing of the spectra

$$E_\pm = \frac{1}{2}\left(E_{2s} + E_{2p_{-1}} \pm \sqrt{(E_{2s} - E_{2p_{-1}})^2 + V^2\mathcal{E}^2}\right), \quad \mathcal{E} = 2\epsilon^3\hbar^4|\vec{E}|/m_\perp^2 e^5, \tag{2}$$

where $V(H) = \langle 2s/\rho e^{i\varphi}|2p_{-1}\rangle$ and the polarization is

$$P_\pm = \pm\mathcal{E}V^2/2\sqrt{(E_{2s} - E_{2p_{-1}})^2 + V^2\mathcal{E}^2}.$$

A graph of $V(H)$ is shown in Fig. 2. Of course, these formulas are valid only when it is possible to neglect the quadratic contributions to the spectrum from other states that are close to the $2s$ and $2p_{-1}$ states; for example, it is necessary that

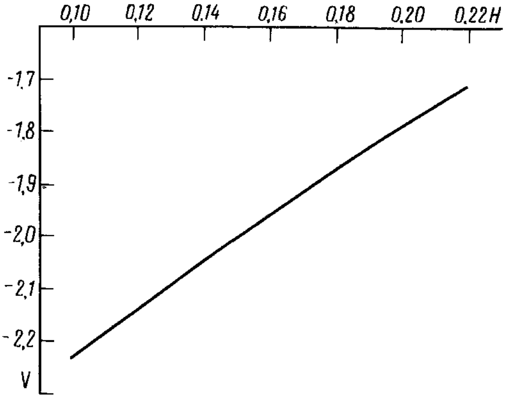

FIG. 2.

$$\mathcal{E}/V \ll |E_{2s} - E_{2p_{+1}}|/ < 2s|\rho e^{-i\varphi}|2p_{+1} >^2 .$$

4. Let us assume that a diode structure made from silicon with a concentration N_d of the order of 10^{16}–10^{17} cm^{-3} of shallow donors is placed in a magnetic field of 99 kOe, whose direction coincides with the principal axis of the crystal and lies in the plane of the *p–n* junction. The electric field in the region of the *p–n* junction, which can be controlled by applying an external voltage, may be of the order of 10^3–10^4 V/cm. Then the level splitting according to Eq. (2) will be 1 meV or less. At a temperature of the order of 1 K one can create different populations $f_\pm$ of the levels $E_\pm$ by using illumination of frequency $\omega = G - E_-$ (G is the band gap). The capacitance of the diode changes because of the redistribution of the charge, and because of the change in the dielectric constant. Without going into the details of possible experiments, we note that this effect

$$\Delta\epsilon/\epsilon \cong (f_+ - f_-)N_d(\hbar^2\epsilon/m_\perp e^2)^3 4\pi V^2/\sqrt{(E_{2s} - E_{2p_{-1}})^2 + V^2\mathcal{E}^2}$$

can be easily detected by capacitance measurements. For the appropriate conditions it can be as large as a few tens of percent.

We thank G. N. Gol'tsman, A. I. Elant'eva, I. B. Levinson, and A. V. Turbiner for helpful discussions.

[1] W. Kohn and J. M. Luttinger, Phys. Rev. **98**, 915 (1955).

[2] N. Lee, D. M. Larsen, and B. J. Lax, J. Phys. Chem. Solids **34**, 1817 (1973); **35**, 401 (1974).

[3] G. L. Bir and G. E. Pikus, *Symmetry and Deformation Effects in Semiconductors* [in Russian], Nauka (1972).

[4] E. M. Gershenzon, G. N. Gol'tsman, and A. I. Elant'ev, Zh. Eksp. Teor. Fiz. **72**, 1062 (1977) [Sov. Phys. JETP **45**, 555 (1977)].

[5] A. V. Turbiner, Usp. Fiz. Nauk **144**, 35 (1984) [Sov. Phys. Usp. **27**, 668 (1984)].

[6] A. V. Turbiner, Yad. Fiz. **46**, 204 (1987) [Sov. J. Nucl. Phys. **46**, 125 (1987)].

[7] I. L. Beinikhes and Sh. M. Kogan, Zh. Eksp. Teor. Fiz. **93**, 285 (1987) [Sov. Phys. JETP **66**, 164 (1987)].

Translated by J. R. Anderson