Influence of the splitting of dislocations on the g factor of holes in a one-dimensional dislocation band

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The electric-dipole spin resonance (EDSR) signal on straight dislocations with equilibrium and nonequilibrium splitting is measured in silicon crystals. It is shown that the g factor of holes in the one-dimensional energy bands corresponding to dislocations depends on the magnitude of their splitting. This result is consistent with the known fact that the energies of the $D3$ and $D4$ dislocation photoluminescence lines depend on the splitting of 60° dislocations. © *1996 American Institute of Physics.* [S1063-7761(96)02510-3]

1. INTRODUCTION

The electronic properties of dislocations in semiconductors are of the fundamental interest because long straight segments of a dislocation can be treated as one-dimensional electronic systems. The number of electrons in one-dimensional dislocation bands can be varied, and the effects associated with them can be investigated by varying the position of the Fermi level in the band gap (by means of doping with small donors and acceptors). Detailed calculations (see Refs. 1–4) show that deformation of the cores of 30° and 90° partials with pairwise closing of the dangling bonds (so-called reconstruction of the dislocation cores) is energetically favorable. The electronic spectrum of a reconstructed dislocation should contain two one-dimensional (1D) bands E_{Dv} and E_{Dc}, which split off from the valence band E_v and the conduction band E_c of the three-dimensional crystal due to the strong deformation of the lattice. Apart from these one-dimensional bands, deep localized electronic states created by defects in the dislocation cores (for example, reconstruction defects containing dangling bonds, steps, etc.) are associated with real dislocations.

It was shown in Refs. 5–7 that the electric-dipole spin resonance (EDSR) signal can be very intense for electrons and holes in one-dimensional dislocation bands, while its intensity is nearly equal to zero for carriers trapped in dislocation defects. Thus, EDSR is a very effective method for investigating one-dimensional dislocation bands. Dislocation EDSR is the one-dimensional version of the "combined" resonance developed theoretically by Rashba (see the review in Ref. 8). It is based on the fact that the term $(\mathbf{V}\times\mathbf{p})\text{-}\mathbf{S}$, which relates the spin degree of freedom of an electron to its momentum $\mathbf{p}$, appears in the electron Hamiltonian when there is no inversion center in the system. As a result, the component $\mathbf{p}_\omega$ of the electron momentum induced by the microwave electric field $\mathbf{E}_\omega$ causes the appearance of an effective magnetic field $\mathbf{h}_\omega=[\mathbf{V}\times\mathbf{p}_\omega]/g\mu_B$, which acts on the electron spin. In the presence of an external static field $\mathbf{H}_0=\hbar\omega/\mathbf{g}\mu_B$, this effective field $\mathbf{h}_\omega$ will excite resonant transitions between the spin levels, which should produce a resonance feature in the dielectric constant $\varepsilon=\varepsilon'+i\varepsilon''$ of the sample; we shall call it EDSR below.

Technically, an ordinary ESR spectrometer is used to observe EDSR, but the sample is placed at the maximum of the microwave electric field, rather than at the maximum of the microwave magnetic field H_ω of the resonator, where it is placed in the case of ESR.

Because of the symmetry properties of a Si crystal, the vector $\mathbf{V}$ is equal to zero for free electrons in the conduction band; therefore, there is practically no EDSR signal for free or weakly bound electrons. However, the local symmetry of dislocations is lower than the symmetry of the crystal, and it does not have an inversion center. Therefore, the magnitude of $\mathbf{V}$ for a deep dislocation state can be very large. On the other hand, in the case of point defects the strong electron localization automatically means that the component $\mathbf{p}_\omega$ induced by the microwave electric field is small. Therefore, at low microwave frequencies (10–40 GHz) the EDSR signal will also be very weak (of the order of or less than the ESR signal). In a one-dimensional (1D) band the situation is totally different. In the direction perpendicular to a dislocation the radius r of the wave function of an electron in this band is fairly small (10–20 Å), and the magnitude of $\mathbf{V}$ is great. On the other hand, the localization length L along a dislocation can be very large and can ensure a large value of p_ω when the field $\mathbf{E}_\omega$ is applied along the dislocation. In this case the EDSR signal can be very intense, exceeding the ESR signal from the same electrons by many orders of magnitude.

According to the calculations in Refs. 6 and 7, the amplitude of the EDSR signal in a 1D band is proportional to the quantity

$$A\propto N(m^*V\mu_\omega S(L/L_D))^2, \tag{1}$$

where L is the localization length of electrons in the dislocation, N is their linear density along the dislocation, and m^* is the electron effective mass. The function

$$S(x)=1-\exp\left(\frac{i\pi}{4}\right)\tanh\left(x\exp\left(-\frac{i\pi}{4}\right)\right)\Big/ x$$

is the structure factor, which takes into account the fact that the field acting on an electron is not equal to the external

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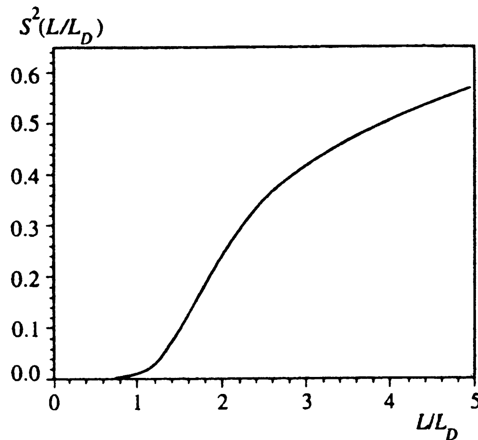

FIG. 1. Calculated dependence of $\mathrm{Re}(S^2(L/L_D))$, which determines the intensity of the EDSR signal, on L/L_D.

electric field due to the polarization of the conducting portion of the dislocation. The parameter L_D, which has the dimensions of length, equals

$$L_D=(e\mu_\omega N\ \ln(L^2/r^2)/\varepsilon\omega)^{1/2}. \quad (2)$$

When L is large, μ_ω has the meaning of the high-frequency mobility of electrons in the one-dimensional band: $\mu_\omega=e\tau/m^*(1+i\omega\tau)$.

Because the multiplier $(\mu_\omega S(L/L_D))^2$ is complex, the EDSR line shape depends on L/L_D. It is similar to the usual absorption curve characteristic of ESR only when $L/L_D<0.5$. When L/L_D is large, the line shape corresponds to a mixture of "absorption" and "dispersion" curves, and when L/L_D increases further, the absorption curve changes sign, i.e., corresponds to a decrease in the microwave conductivity of the sample at resonance. Thus, a computer analysis of the line shape permits an independent determination of L/L_D.

The intensity of the EDSR signal is very strongly dependent on the electron localization length L (see Fig. 1). Taking the value $N\approx5\times10^5$ cm^{-1} for N and setting $\mu_\omega\approx100$ cm^2/V·s, we obtain a value of L_D of order 0.1 μm. This means that an intense EDSR signal can be expected only for linear segments of dislocations with a length L greater than 1000 Å. This assertion correlates with the experimental fact that EDSR signals from both electrons[9] and holes[10–12] in Shockley dislocations are observed only when a special plastic deformation procedure, which ensures the generation of long straight segments of screw and 60° dislocations, is used. This technique, which was developed by H. Alexander,[13,1] is based on the fact that dislocations introduced during plastic deformation at $T>700$ °C subsequently straighten out due to the application of a high load to the sample at T of order 400 °C and cooling of the samples to room temperature without removing the load. Annealing such samples for $T>500$ °C causes the dislocations to bend under the action of the internal fields of elastic stresses. It was shown in Ref. 12 that the EDSR signal vanishes in this case due to the sharp decrease in the localization length L of the carriers in one-dimensional dislocation bands.

Low-temperature deformation under a high load not only results in straightening of the dislocations, but also causes the magnitude of their splitting $\mathbf{d}$ (i.e., the width of the packing defect separating the 30° and 90° Shockley partials that form the complete 60° dislocation) to differ from the thermodynamic-equilibrium value.[1,13] In this case there should be a change in the form of the potential well responsible for the formation of the one-dimensional dislocation band, which can influence the g factor of the holes in it. The purpose of the present work is to experimentally test this assertion using EDSR.

2. SAMPLES AND EXPERIMENTAL METHOD

Silicon single crystals grown by vacuum crucible-free zone melting (FZ-Si) and doped with bromine to a concentration equal to 3×10^{15} cm^{-3} were deformed to 0.5% by compression at 820 °C under a 35 MPa load. The compression axis was deflected 10° from the [110] direction by rotation about the [1,−1,0] direction. In this geometry dislocations were introduced predominantly in the (111) slip plane with [−1,0,1] and [0,−1,1] Burgers vectors. The dislocation density was of the order of 3×10^7 cm^{-2}. After high-temperature deformation, the sample was cooled to 420 °C, and a 180 MPa load was applied to it for 15–20 min. Then the sample was cooled to room temperature without removing the load. This resulted in the appearance of loops consisting of straight screw and 60° dislocations in the [1,−1,0], [−1,0,1], and [0,−1,1] directions.

An ESR spectrometer with a working frequency of 9300 MHz and a rectangular resonator was used to observe the EDSR signal. The sample was placed at the maximum of the microwave electric field $\mathbf{E}_\omega$ of the resonator. Modulating the magnetic field $\mathbf{H}_0$ with an amplitude of 10 Oe and a frequency of 130 Hz made it possible to record the derivative of the absorption signal $d\varepsilon''/dH_0$ using a lock-in amplifier. The measurements were performed at 6.5 K. The sample was illuminated by a miniature incandescent lamp fastened to the resonator, which was placed together with the sample in a continuous flow He cryostat.

The dislocation photoluminescence spectra were recorded at 4.2 K by a germanium photocell. The photoluminescence was excited by an argon laser, the excitation power being equal to 10 mW/mm^2.

3. EXPERIMENTAL RESULTS AND DISCUSSION

The EDSR spectrum of holes in Shockley dislocations consists of two groups of lines, Si-KC1 and Si-KC2 (see Ref. 11). The Si-KC1 lines have widths from 180 to 700 Oe and values of L/L_D determined from the line shape from 1.6 to 6, while the Si-KC2 lines are narrower (from 80 to 200 Oe) and are characterized by a smaller value of L/L_D (from 0.9 to 2). There is still no unequivocal explanation for the presence of two groups of lines. It has not been ruled out that one group is due to 60° dislocations and the other group is due to screw dislocations. However, other alternatives are possible.

Figure 2 illustrates the variation of L/L_D and the intensity of the EDSR line as the optical illumination of the sample is increased for a Si-KC2 line (curves *1*) and for a

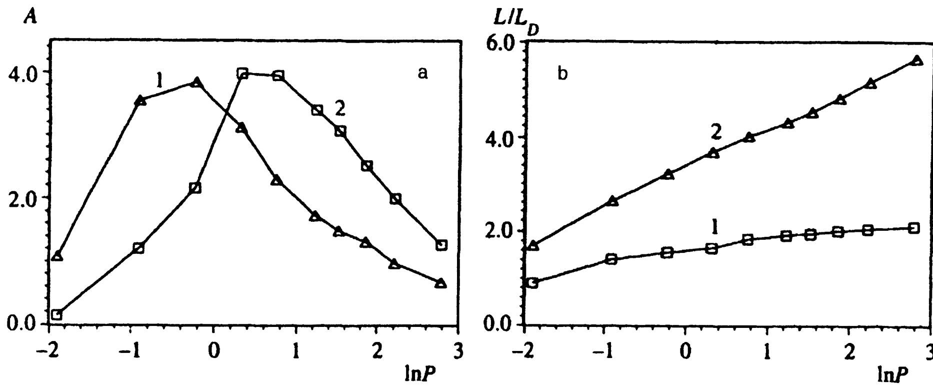

FIG. 2. Dependence of the intensity of the EDSR line (a) and L/L_D (b) on the natural logarithm of the power of the optical illumination of the sample (in relative units): curves *1* — for a Si-KC2 line, curves *2* — for a Si-KC1 line.

Si-KC1 line (curves *2*). As the light intensity increases, the EDSR signal at first increases and then decreases, while the value of L/L_D increases monotonically. Such behavior is associated with the variation of hole density N in the one-dimensional E_{Dv} band upon illumination. In the absence of illumination, a dislocation in a p-type sample is positively charged by the holes trapped in the one-dimensional E_{Dv} band. This results in Coulomb warping of the bands about the dislocation of order

$$e\Phi = 2e^2 N \ln(\lambda N)/\varepsilon, \tag{3}$$

where ε is the dielectric constant of silicon, e is the charge of the electron, N is the linear hole density in the dislocation, and λ is the shielding radius [for $e\Phi \gg kT$, it is of order $\lambda = (N/\pi p)^{1/2}$, where p is the concentration of free electrons or shallow acceptors, $p = 3\times 10^{15}$ cm^{-3}]. In the presence of nonequilibrium photoexcited electrons at low temperatures, N is determined by the balance between the hole and electron trapping rates:

$$dN/dt = pr_h v_{\rm th} \exp(-e\Phi/kT) - nr_e v_{\rm th}, \tag{4}$$

where n and p are the concentrations of free electrons and holes, r_e and r_h are the capture radii of electrons and holes, respectively, in a neutral dislocation, and $v_{\rm th}$ is the thermal velocity of the free electrons and holes. The first term in Eq. (4) corresponds to hole capture, and the second term corresponds to electron capture. (At low temperatures their thermal activation with the dislocation can be neglected even under weak illumination.) Hence we obtain

$$N \approx \varepsilon kT \ln(pr_h/nr_e)/6e^2. \tag{5}$$

As the incident light intensity is increased, the value of n/p increases, tending to unity. This causes a decrease in N due to the small probability of hole capture by a positively charged dislocation in comparison with electron capture. At first glance, a decrease in N should lead to a decrease in L_D proportional to $N^{1/2}$ [see Eq. (2)] and, accordingly, to an increase in L/L_D. For $L/L_D > 1.8$–2, the structural multiplier $S(L/L_D)^2$ in Eq. (1) depends weakly on L/L_D (see Fig. 1), and as N decreases, the intensity of the EDSR signal actually decreases (see Fig. 2). However, at small values of L/L_D the function $S(L/L_D)^2$ depends on N approximately as N^{-2}, and an increase in the intensity of the EDSR signal is observed despite the decrease in N.

As is seen from Fig. 2, the ratio between the intensities of the Si-KC1 and Si-KC2 lines depends on the illumination intensity. Therefore, to measure the anisotropy of both groups of lines we used two different levels of illumination. A second complication arises because the EDSR signal vanishes when the electric field $\mathbf{E}_\omega$ is perpendicular to the direction of the dislocation. Therefore, the g-factor anisotropy was measured using two geometries: $\mathbf{E}_\omega$ parallel to the magnetic field $\mathbf{H}_0$ and $\mathbf{E}_\omega$ perpendicular to $\mathbf{H}_0$. This made it possible to observe the EDSR signal at all angles of orientation of the sample relative to the magnetic field.

Figure 3 plots the dependence of the g factor of various lines on the angle between the magnetic field and the $[1,-1,0]$ direction of the sample as it is rotated about the

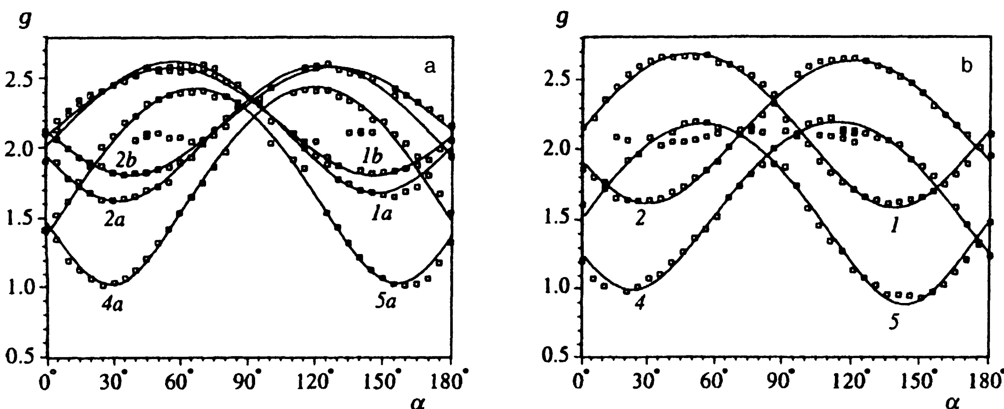

FIG. 3. Dependence of the g factor of EDSR lines on the angle α between the magnetic field $\mathbf{H}_0$ and the $[1,-1,0]$ direction of the sample as it rotates about the $[1,1,-2]$ axis: a — sample immediately after deformation, b — same sample after annealing for 20 min at 350 °C.

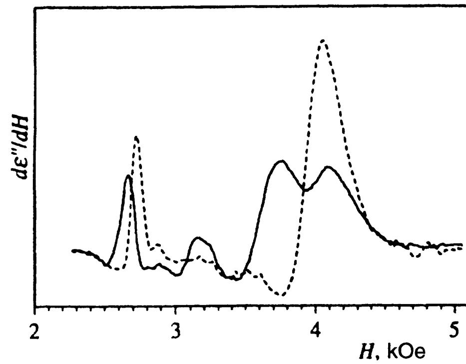

FIG. 4. EDSR spectra at $T=6.5$ K under illumination corresponding to $\log P=1.2$ in Fig. 2: solid curve — before annealing, dashed curve — after annealing of the sample for 20 min at 350 °C. The Si-KC2 lines dominate in the spectrum at the illumination power cited.

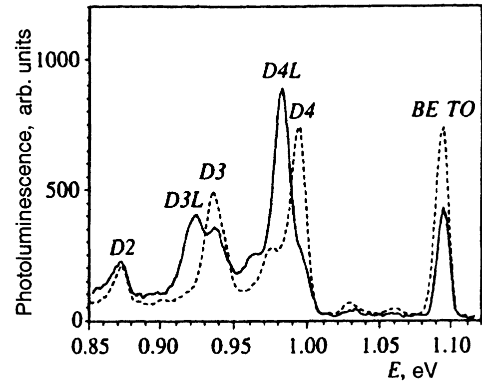

FIG. 5. Photoluminescence spectra of a sample before (solid curve) and after (dashed curve) annealing for 20 min at 350 °C, $T=4.2$ K.

[1,1,−2] axis. Figure 3a corresponds to a sample immediately after deformation, and Fig. 3b corresponds to the same sample after annealing for 20 min at 350 °C. Lines *4*, *4a*, and *4b* correspond to the Si-KC1 group, while lines *1*, *2*, *1a*, *1b*, *2a*, and *2b* correspond to the Si-KC2 group. It is seen that such gentle annealing drastically altered the positions of several lines in the EDSR spectra. The g-tensor parameters of lines *4a* and *5a* varied appreciably as a result of the annealing (they went over to *4* and *5*). While the experimental values of the g factor for lines *4a* and *5a* before the annealing were 1.02 and 2.41, after the annealing they became 0.95 and 2.2. The principal axes of the g tensor also shifted by several degrees. However, the most appreciable changes occurred in the Si-KC2 lines, i.e., their number decreased from two pairs to one. The g-tensor parameters of lines *1a* and *2a* are fairly close to the parameters of lines *1* and *2* in the annealed sample, while lines *1b* and *2b* simply went over to lines *1* and *2* after the annealing. This is illustrated by Fig. 4, where the solid curve shows the EDSR spectrum of the Si-KC2 lines before the annealing, and the dashed curve shows the spectrum after annealing.

According to electron-microscopic data, annealing the sample at 350 °C does not result in appreciable changes in the morphology of the dislocations. They remain straight as before, and their density and type remain unchanged. However, before the annealing all the 60° dislocations can be divided[1,13] into three groups according to the value of their splitting parameter d: a) $d\approx d_0$, b) $d<d_0$, and c) $d>d_0$. Annealing at 300–350 °C causes the splitting of all the dislocations to achieve the thermodynamic-equilibrium value d_0 (see Ref. 14). The gentle annealing indicated also causes changes in the positions of the $D3$ and $D4$ dislocation photoluminescence lines.[14] Figure 5 presents the photoluminescence spectra of a sample that we measured before (solid curve) and after (dashed curve) annealing. There is presently no doubt that the $D4$ line corresponds to no-phonon recombination on 60° dislocations, and the $D3$ line is the TO phonon replica of the $D4$ line.[14–17] Thus, the variation of the energy of these dislocations directly correlates with the variation of their splitting. As is seen from Fig. 5, photoluminescence corresponding to both the equilibrium splitting d_0 of the dislocations (the $D3$ and $D4$ lines) and splitting with $d<d_0$ (the $D3L$ and $D4L$ lines) is observed. The annealing results in the disappearance of the photoluminescence lines corresponding to small splitting. This correlates with the disappearance of EDSR lines *1b* and *2b* in Fig. 3.

Thus, EDSR lines *1a* and *2a* in the unannealed samples can be associated with dislocations which have nearly equilibrium splitting, and lines *1b* and *2b* can be associated with dislocations with small splitting. The physical explanation of the dependence of the g factor on the splitting of the dislocations is as follows: the potential for a hole near a split dislocation consists of two troughs parallel to one another. In the case of a 60° dislocation one of them corresponds to a 30° partial, and the other corresponds to a 90° partial. It is clear that the energy at the bottom of the one-dimensional energy band appearing in response to the presence of this potential should depend on the distance d between the partials because of the interference between the potential troughs of the partials. The smaller the splitting d, the deeper the bottom of the one-dimensional band should be. This is observed in the photoluminescence spectra, where a small radiated energy corresponds to dislocations with a small value of d. The wave function of a hole in the 1D band should, of course, depend on the form of the potential. Because of the strong spin-orbit interaction for holes, their g factor depends strongly on the form of the wave function and consequently depends on the magnitude of the splitting.

The question of why photoluminescence lines corresponding to dislocations with $d>d_0$ are not observed in the samples investigated naturally arises. One of the explanations is that such dislocations possibly have large point defects. As a result, there is no EDSR signal because of the small localization length and (or) because all the holes in such dislocations are trapped in the deeper states corresponding to these defects. On the other hand, there is no photoluminescence from such dislocations due to the strong competition on the part of the nonradiative recombination through the deep point defects.

Thus, unlike the known point defects, for which the g tensor has a steady tabulated value, in the case of dislocations the g-tensor parameters depend on the sample history and the plastic deformation regime.

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