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EPR line width and spin-relaxation rates of shallow and deep donors in isotopically controlled silicon

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Abstract

The results of a numerical calculation of the contribution of ligand superhyperfine interactions to the line width for the phosphorus donor electron in silicon are reported and show linear behavior at lower concentrations compared to deep centers. The linear dependence for the phosphorus center in silicon predicts an electron spin-relaxation time for isotopically purified ^{28}Si:P longer than expected on the basis of the common square-root law. The confrontation of line width in deep-level centers with shallow states confirms that the behavior depends on the distribution of spin density around the paramagnetic center.

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1. Introduction

At present there is again a great interest in the relaxation processes in spin systems since it is connected with the development of spintronics and perspectives of building quantum computers on the basis of ^{28}Si:P or GaAs quantum dots [1]. Silicon differs advantageously from GaAs by the fact that the enrichment of silicon by the ^{28}Si isotopes makes it a spinless material. Therefore, in case of silicon quantum computer models the condition of spin coherency at quantum operations can be realized easier than for GaAs which is caused by a significant increasing of spin-relaxation time and spin-dephasing time at the isotopic enrichment.

In Ref. [2] we reported about linear dependencies of the superhyperfine interaction contribution of the electron localized on the intrinsic vacancy defect (V^-) and the iron impurity (Fe^+) in silicon to the EPR line width on the concentration of ^{29}Si nuclei having nonzero spin. This behavior is caused by changing of the hyperfine fields shift distribution from Gaussian to Lorentzian. It is well known that interaction of electron spins with nuclear spins gives the most significant contribution to the spin-relaxation rate at low temperatures. Therefore, the enrichment of silicon by isotopes with zero nuclear spin and taking into account the linear contribution of superhyperfine interaction to the line width will give less contribution to the spin-relaxation rate compared to other relaxation processes. In contrast to centers with deep levels the wave function of the phosphorus donor electron in silicon interacts with many nuclei. Therefore, it is not possible to predict results in advance without computation of the contribution of the ligand superhyperfine interactions to the line width for the phosphorus donor electron in silicon. In this work we present results of such calculations.

2. Numerical calculation of the ^{29}Si ligand superhyperfine interactions contribution to the line width

There is an existing opinion in the literature that the contribution of the ligand superhyperfine interactions to the line width for paramagnetic centers in solids has a

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square-root behavior (see, e.g. Refs. [3,4]). In Ref. [5] we suggest such a behavior for phosphorus shallow donors in silicon in contradiction to the deep centers reported in Ref. [2]. Using the methods described in Ref. [2] we calculated the contribution of the ligand superhyperfine interactions to the line width for the phosphorus donor electron in silicon. For calculations the superhyperfine constants for the phosphorus center in silicon obtained by electron–nuclear double resonance (ENDOR) in Ref. [6] were used. For improvement of the previous results we have taken into account the changing of the line shape with changing of nuclear concentration by applying deconvolution methods for finding the inhomogeneous contribution of the superhyperfine interaction to the calculated line shape. We used the idea of the works of Posener [7] and Stoneham [8] for numerical calculation of the convolution of the initial absorption line shape which was chosen Lorentzian and superhyperfine broadening which is Gaussian at high and medium concentrations of nuclei.

The convolution of the two line shapes could be expressed as [7]

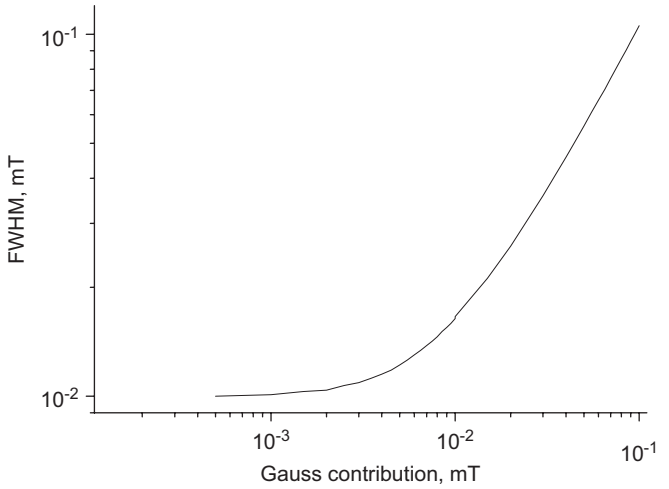

Fig. 1. Dependence of the convoluted line width on the width of the Gaussian distribution ${}^{G}\Delta H_{1/2}$ with a constant Lorentz contribution ${}^{L}\Delta H_{1/2} = 0.01\,\mathrm{mT}$.

$$Y(H-H_0) = \frac{(\ln 2)^{1/2}}{\pi}\frac{{}^{L}\Delta H_{1/2}}{{}^{G}\Delta H_{1/2}}\int_{-\infty}^{\infty}\frac{e^{-x^2}\,dx}{\left(\frac{{}^{L}\Delta H_{1/2}}{{}^{G}\Delta H_{1/2}}\right)^2 \ln 2 + [2(\ln 2)^{1/2}((H-H_0)/{}^{G}\Delta H_{1/2}) - x]^2}, \quad (1)$$

where ${}^{L}\Delta H_{1/2}$ and ${}^{G}\Delta H_{1/2}$ are the full widths at half maximum (FWHM) for Lorentz and Gauss lines correspondingly. Since the Lorentzian contribution is known and was chosen constant (we used a value of the initial line width of 0.01 mT, much smaller than in the previous paper [2]) we could calculate the Gaussian contribution to the line shape. For this aim we made the integrations in Eq. (1) at different values of ${}^{G}\Delta H_{1/2}$ and obtained the dependence of the line width of the Lorentz and Gauss line shapes convolutions on the Gaussian contributions. The results are shown in Fig. 1. From this dependence we could derive the Gaussian contribution of the superhyperfine interaction to the line width using the algorithm of calculations as in Ref. [2]. As can be seen from the calculated dependencies of the width (FWHM) of resonance lines for phosphorus and iron (Fe^+) centers in silicon represented in Fig. 2 the line width decreases linearly under decrease of concentration of ^{29}Si magnetic nuclei below some small but different concentrations for deep and shallow centers. In the range of high concentrations ($>3\%$ for P- and $>10\%$ for Fe^+-center) the dependencies obtain a square-root character. It is seen that the deconvolution is mostly effective at some range of nuclear concentrations below 5%. It is negligible at very low concentrations, where there is a Lorentz contribution to the Lorentz line shape and at high concentrations where large Gauss and small Lorentz parts contribute to the convolution of the line shapes. This can be confirmed by using experimental data on superhyperfine tensors for phosphorus and iron in silicon. One can calculate the sums of a_k^2, a_k^4 and $a_k^2 a_j^2$ (in formulas (9) and (10) of Ref. [2]) and obtain the ratios of fourth and second moments. The changes of ratios $M_4/3M_2^2$ for phosphorus and iron centers in silicon are shown in Fig. 3. Again one can see the line shape transformation from Lorentzian to Gaussian type for the phosphorus center as well as for iron when the concentration of ^{29}Si nuclei increases.

For the iron center there is a dip around 4% of concentration which was not mentioned in the earlier paper [2] and which appeared because we used for calculations a smaller width ${}^{L}\Delta H_{1/2} = 0.01\,\mathrm{mT}$ of the initial line and which arises from the fact that only a small number of isotropic hyperfine constants were measured in the ENDOR experiment for the Fe^+ center [9] which leads to unsmoothness of the line shape (Fig. 4). This dip was only slightly decreased after the deconvolution procedure. To examine this dip in more detail we used for calculations also anisotropic hyperfine constants in addition to isotropic ones. In this case resonance fields were calculated using the first-order perturbation formula which included the hyperfine interaction constants for the ith nucleus with the paramagnetic center: isotropic a_i and anisotropic b_{ik}, where k enumerates interactions with all atoms in the shell:

$$B_{\mathrm{sh},z} = B_{0,z} + \Sigma_{ik} m_{I,i}(a_i + b_{ik,z})/g\mu_B, \quad (2)$$

where B_0 is the center of resonance line, without hyperfine shift, B_{sh} is the field with hyperfine shift, $m_{I,i}$ is the projection of spin of the ith nucleus on the direction of magnetic field, g value is the spectroscopic splitting factor. One can see in Fig. 4 that adding of the anisotropic hyperfine constants for iron in silicon essentially affects the