Spin Relaxation of Electrons Localized on Shallow and Deep Donor Centers in Silicon with Different Isotopic Composition

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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 spin-lattice relaxation processes in chromium doped silicon samples enriched by ^{28}Si isotope and with natural isotopic abundances were studied.

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Nowadays the relaxation processes in spin systems are again of a great interest because of spintronic development and perspectives for building the 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 spin coherency at quantum operations can be realized easier than for GaAs ones. It is caused by a significant increasing of spin relaxation time and spin dephasing time at the isotopic enrichment. The use of isotopically enriched crystals leads to the possibility to investigate a number of new effects in relaxation processes. One of them is the predicted linear dependence of the superhyperfine interaction contribution of the electron localized on the intrinsic vacancy defects (V^-) and the iron impurities (Fe^+) in silicon to the EPR line width on the concentration of ^{29}Si nuclei possessing nonzero spin [2]. It is well known that the influence of interaction between electron and nuclear spins on the spin relaxation rate is more significant at low temperatures. The enrichment of silicon by isotopes with zero nuclear spin and the linearity of superhyperfine interaction contribution to the line width will decrease the influence of superhyperfine interaction on the spin relaxation rate in comparison with other relaxation processes.

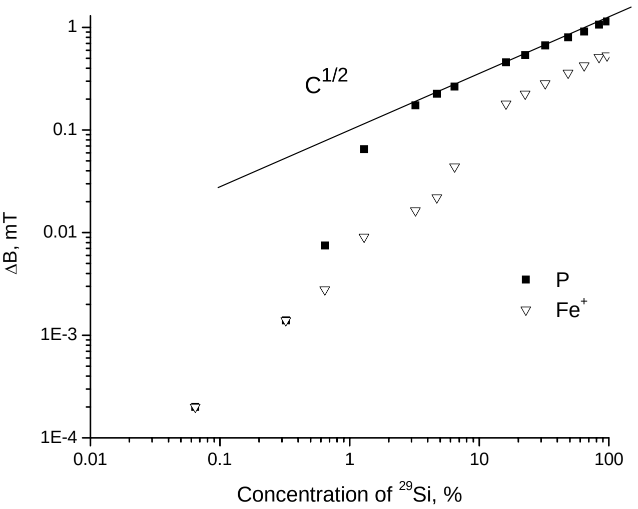

Fig.1. Dependence of the full width at half maximum (FWHM) of P and Fe^+ centers EPR lines in silicon on concentration of magnetic nuclei ^{29}Si.

There is an opinion in the literature that the contribution of the ligand superhyperfine interactions to the line width for paramagnetic centers in solids has a square- root behavior. In Ref. [3] we suggested such a behavior for phosphorus shallow donors in silicon in contradiction to 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. In these calculations the superhyperfine interaction constants for the phosphorus center in silicon obtained by electron-nuclear double resonance (ENDOR) in Ref. [4] were used. To improve the results we have taken into account the changes in the line shape for different nuclei concentration by applying the deconvolution methods for finding the inhomogeneous contribution of the superhyperfine interaction to the calculated line shape. As it can be seen in Fig.1 the calculated dependence becomes linear at concentrations of magnetic nuclei below 3%. Hence, in case of shallow donor center the deviation from square root law can be also obtained, but at a lower concentration in comparison with the deep centers. More rapid linear behavior of this dependence leads to longer times of spin system dephasing at isotopic enrichment with zero spin isotope of silicon. The line widths measured for phosphorus in monoisotopic silicon-28 samples show a great dispersion of values (0.022 mT [4], 0.008 mT [5], 0.045 mT [3]). It means that measured values depend on the history of samples and therefore on the additional relaxation mechanisms. Among them it could be combined spin-spin and spin-lattice relaxation with participation of other defects. We studied spin-lattice relaxation processes in chromium doped silicon samples enriched by ^{28}Si isotope and with natural isotopic abundances.

From the temperature dependencies of the EPR line width and continuous saturation experiments we obtained spin-lattice relaxation rates in the wide temperature range for silicon samples with different isotopic composition doped by chromium. We investigated samples of monoisotopic silicon (^{28}Si-99.873%, FZ-grown) doped by chromium at the range of concentrations $2.5 \cdot 10^{15}$ – $1.5 \cdot 10^{16}$ cm^{-3}, and samples of natural silicon (Chohralsky grown) with chromium ions concentration $2 \cdot 10^{15}$ – $8 \cdot 10^{15}$ cm^{-3}. The temperature dependencies of chromium ion spin-lattice relaxation rate (T_1^{-1} (T)) are shown in Fig.2.

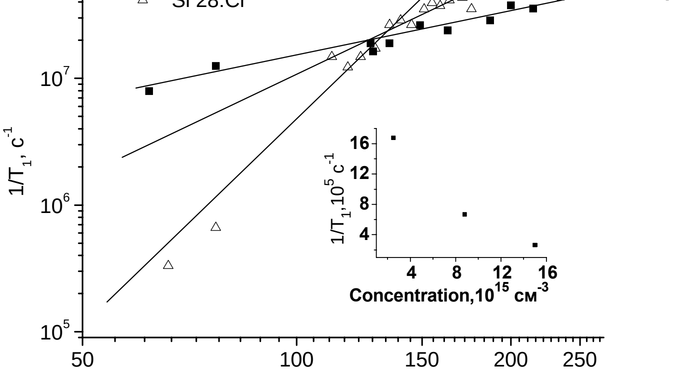

Fig.2. Temperature dependencies of chromium ions Cr^+ spin-lattice relaxation rate in silicon with different isotopic composition.

To explain the obtained temperature dependencies of the spin-lattice relaxation rate for silicon doped by chromium we have considered spin-relaxation model represented in Fig.3. For monoisotopic silicon-28 sample for investigated temperature range the obtained dependence can be described by Bloum-Orbach relaxation process [6] (Fig. 4a). In this case it is enough to take in account only the relaxation channel “Spin A – phonons – thermostat” and neglect “phonons – thermostat” energy transfer time to fit the dependence (T_1^{-1} (T)). But for samples with natural isotopic composition the dependencies couldn’t be correctly described by only one relaxation process. For less chemically and isotopically purified samples one needs to consider additional relaxation channels, such as “Spin A – Spin B – phonons – thermostat”. The second channel may be more effective than the first one only if spins “B” transfer their energy to the phonon subsystem faster than “A” spins. However, as the “Spin A – Spin B” interaction is a dipolar one and has characteristic time of interaction, the mentioned relaxation channel is effective only in the temperature range, when dipole-dipole interaction time is shorter than “Spin B – phonons” energy transfer time. In this case, the spin-lattice relaxation rate can be expressed as:

$$(T_A)^{-1} = \left(\frac{(T'_{12} + T''_{12})^{-1}}{\gamma'(2\pi)^2 \Delta\nu^2_{dip}} + \frac{1}{(T'_{12} + T''_{12})^{-1}} \right)^{-1} + (T_1 + T'_1)^{-1} \qquad (1)$$

where (T_{12}''), $(T_1')^{-1} \sim \alpha T$ are the phonons transfer rates, $(T_{12}')^{-1}$, $(T_1)^{-1}$ are the spin-phonon energy transfer rate, γ' is the gyro-magnetic ratio, $\Delta\nu^2_{dip}$ is the dipole-dipole contribution to the line width. For the samples of natural isotopic composition the dependence of spin-lattice relaxation rate at T higher than 77 K has a linear behavior. The relaxation rate at high temperatures is defined mostly by phonons transfer rate and in the quasidiffusion regime one has a linear law [7]. The results of fitting are shown in Fig. 4b. For low temperature range the parallel channel of relaxation via dipole interaction with spins “B” becomes more effective. To explain the value of relaxation rate at 10K it was necessary to take in account Orbach processes that can serve as evidence of complicated multilevel electronic structure of center B.

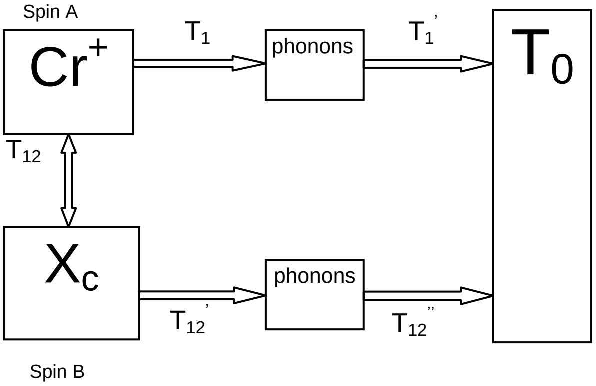

Fig.3. Model of spin relaxation processes

One can believe that the parallel channel of relaxation could be a cause of obtained spin-lattice relaxation rate dependence on the concentration of chromium ions in the monoisotopic silicon samples (insert in Fig.2), for which the concentration of chromium ions is comparable with that one of “B” spins. The interaction of chromium ions with these centers increases the effectiveness of spin-lattice relaxation. When concentration of “B” spins is lower than chromium ions concentration only small part of “B” spins relaxes effectively. The influence of this part is negligible in comparison with more durable spin-lattice relaxation of major part of ions which don’t interact with impurity. Oxygen concentrations in investigated samples are 10^{18} cm^{-3} (natural silicon) and 10^{15} cm^{-3} (monoisotopic silicon), thus it is naturally suppose that “B” spin is a center bound with oxygen, spin-lattice relaxation rate of which is higher than that one of chromium ions.

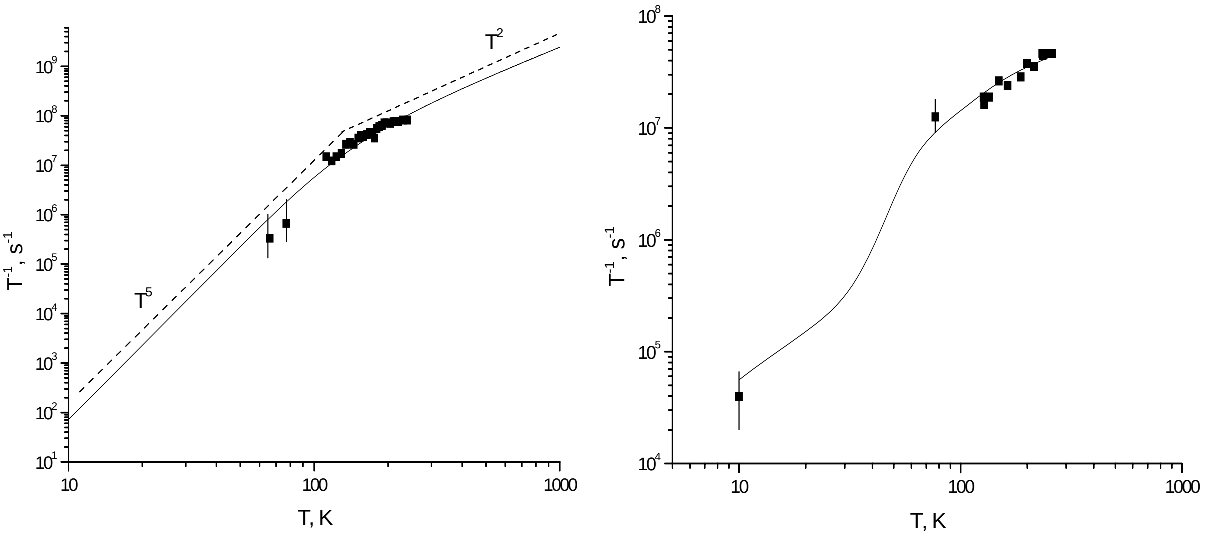

Fig.4. Dependencies of spin-lattice relaxation rate for chromium ions Cr$^+$ on temperature in isotopicaly enriched (a) and natural (b) silicon. The solid line represents the results of fitting.

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