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Spin relaxation times of donor centers associated with lithium in monoisotopic ^{28}Si

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Abstract. We report a detailed study of electron longitudinal and transverse spin relaxation times for Li donors in monoisotopic ^{28}Si over the temperature range 4–20 K using continuous wave and pulsed electron paramagnetic resonance. Comparison of the obtained spin-lattice relaxation times for the states of the isolated donor center and lithium complex LiO showed that due to the presence of orbital degeneracy, relaxation is faster for single lithium than for the LiO complexes with the nondegenerate ground state. For the isolated lithium center in silicon the relaxation is well described by Blume-Orbach process, with the parameters of the spin-orbit coupling $\sim 1 \cdot 10^{-6}$ meV, compare to Orbach process for LiO complex with spin-orbit coupling parameter $\sim 1.5 \cdot 10^{-2}$ meV.

Introduction

For applications based on the spin-dependent phenomena the spin-lattice relaxation times are the important parameters. The spin relaxation for Group-V shallow donor spins in Si crystals is well described by the Orbach processes due to transitions between the ground singlet state and spin-orbit split excited triplet state [1]. Lithium is another shallow donor in silicon which occupies interstitial position and has an inversion structure of levels with the five-fold degenerate ground state (triplet and doublet), that makes it perspective for more flexible manipulation of spin states in promising applications of spintronics and quantum computation. There are several families of electron paramagnetic resonance (EPR) spectra which can be attributed to isolated Li donor center: with $g > 2.000$, that were observed in classical work [2] of G. Watkins and F.S. Ham in silicon with natural composition of isotopes, and $g < 2.000$ of both lithium related centers in monoisotopic ^{28}Si crystals, that were recently reported in our works [3,4]. Two different sets of g -values are described by very different (up to three orders of magnitude) parameters of spin-orbit (SO) coupling [3]. Study of the spin-lattice relaxation of electrons localized on Li and LiO centers, allows one to estimate independently the constants of the SO interaction.

Here we report a detailed study of longitudinal T_1 and transverse T_2 spin relaxation times for Li related shallow donors in monoisotopic ^{28}Si over the temperature range 4–20 K using continuous wave (CW) and pulsed EPR techniques. The investigation is concerned with mechanisms which may be responsible for spin relaxation of isolated lithium donor with $g < 2.000$ and LiO complex in monoisotopic ^{28}Si crystals.

Experimental

The measurements were done on lithium diffusion doped ($\sim 10^{16} \text{ cm}^{-3}$) samples of floating zone grown monoisotopic ^{28}Si (99.994% of major isotope) with the oxygen content $\sim 2 \cdot 10^{14} \text{ cm}^{-3}$. The spin

spin-lattice relaxation times were determined from the dependences of the saturation factor of the resonance lines on the microwave magnetic field in the sample in the temperature range of 4 - 20 K, as well as by pulse methods at 6 K (X-band) and 15 K (W-band). The measurements were performed on Bruker EMX-plus spectrometer using helium cryostat ER 4112 HV and Bruker-Elexsys spectrometers at X- and W-band (9.6 and 94 GHz) EPR spectrometers.

Results and discussion

EPR spectra of Li-doped single crystal of monoisotopic ^{29}Si recorded at $T = 4$ K contain lines of the LiO center with a well resolved structure related to the triplet and doublet states (Fig. 1(a)). As the temperature increases from 4 to 10 K the EPR spectrum of lithium is superimposed by the spectrum with trigonal symmetry of the electron localized on LiO bond, which consists of four hyperfine structure lines according to the interaction with ^7Li nuclear spin $3/2$ (Fig. 1(b)).

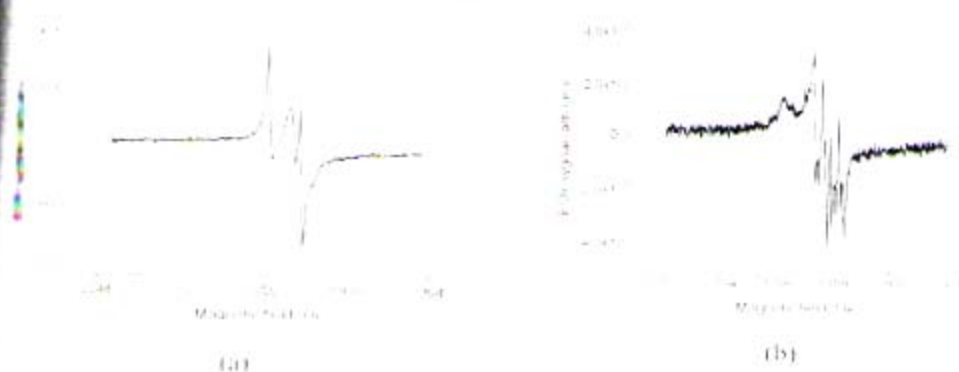


Fig. 1. EPR spectra in lithium doped ^{29}Si sample at zero applied stress, $\mathbf{H} \parallel [100]$. (a) - LiO and Li lines of lithium $g = 2.000$ center at $T = 4$ K, (b) - Li line of lithium center and four ^7Li hyperfine lines of LiO center at $T = 10$ K.

Comparing the EPR spectra taken at different temperatures we can draw several conclusions. Firstly, LiO spectrum is not observed at a low temperature, due to longer times of spin relaxation as compared with Li and it is saturated at low power of microwave field. Secondly, the intensity of Li EPR spectrum rapidly decreases with increasing temperature from 4 to 10 K, while the line of the LiO center observed at higher temperatures (10 - 20 K), which confirms the fact that the energy spectrum of centers differs significantly. This is consistent with the optical spectra [5] indicating that the nearest excited state (A_1) above the ground state of Li ($E_1 - T_1$) is 1.8 meV, and the distance between the ground state A_1 and excited state ($E_1 - T_1$) for the LiO center is 7.7 meV.

The spin-spin T_2 and spin-lattice T_1 relaxation times were determined from the dependences of the saturation factors of the resonance lines on the microwave magnetic field in the sample in the temperature range of 4 - 20 K by the following expression:

$$\frac{1}{S} = 1 + \frac{1}{4} \gamma^2 H^2 T_1 T_2 \quad (1)$$

The dependences of the saturation factor on the microwave field for the T_2 and T_1 components of the spectrum of lithium and for LiO complex are shown in Fig. 2. As can be seen, such dependence for T_2 component of the spectrum is not linear, unlike the rest of the lines of the spectra. Two slopes of the dependence indicate that the process is described by two sets of the relaxation times ($T_1 = 1.2 \cdot 10^{-4}$ and $1 \cdot 10^{-5}$ s for T_2 component and $6 \cdot 10^{-5}$ s for T_1) due to the inhomogeneous distribution of lithium in silicon samples. This is confirmed by the fact that there is a broad base of the line corresponding T_2 component of the spectrum due to the superposition of the

spectrum with the line of a greater linewidth. This broadening can be caused by defects located in the surrounding of lithium center [6].

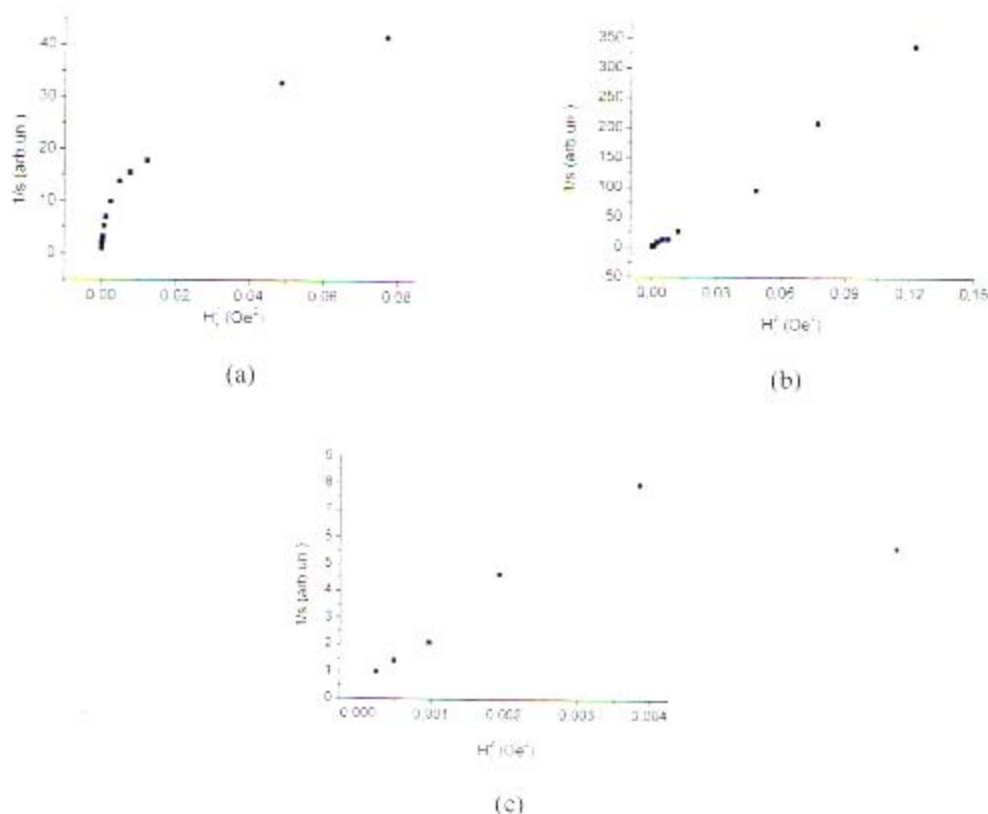


Figure 2. Dependences of the saturation factor on the microwave magnetic field in the sample for (a) T_z and (b) T_{xy} components of the lithium spectrum at $T=4K$ and (c) – for LiO spectrum at $T=10K$, $H \parallel [100]$.

From the obtained dependences of the saturation factor on the microwave magnetic field were determined the spin-spin and spin-lattice relaxation times. Measured T_2 times are 6.5×10^{-7} and 4.8×10^{-7} for LiO spectrum and the T_z component of the Li spectrum, respectively.

Since with temperature increasing E and T_{xy} components of EPR spectra overlap with the line of LiO complex the temperature dependences of the spin-lattice relaxation time are shown only for the T_z component. At 6 K the spin-lattice relaxation times were obtained by pulse methods, at remaining temperatures we used the method of saturation of the CW EPR lines (Fig.3). It can be seen that results obtained by both methods are in good agreement for the LiO complex. At temperatures 4 K and 6 K spin relaxation times for T_z component of the lithium spectrum do not correspond to the dependence behavior at higher temperatures. Indeed, method of CW saturation shows higher values of the spin relaxation rate because due to the nonuniform distribution of lithium the most slowly relaxing centers already saturated and do not contribute to measured signal. If the saturation is pulsed, due to the application of short pulses the spectrum excitation band is greater than the range of fields in which there are lines of the entire spectrum. Therefore it is impossible to determine accurately which state corresponds to the measured relaxation time.

Comparison of the obtained spin-lattice relaxation times for the states of the isolated donor center and the LiO complex which have a different structure of the ground states showed that due to

presence of the orbital degeneracy, relaxation is faster for single lithium than in the complexes with oxygen, for which the ground state is not degenerate [5].

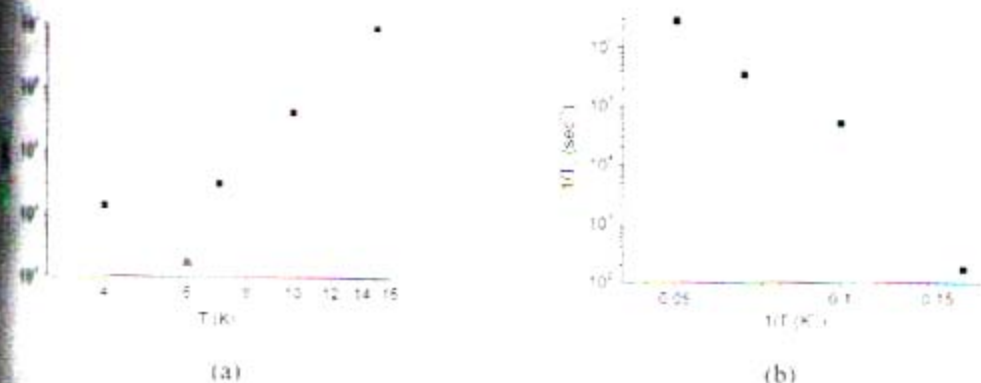


Fig. 3. Temperature dependences of the spin-lattice relaxation rates for T_1 component of the EPR spectrum (a) and LiO (b). [100]. The solid lines denote the Blume-Orbach and Orbach approximations, respectively.

For the isolated lithium impurity the relaxation rate as a function of temperature T is well described by the Blume-Orbach process [7],

$$\frac{1}{T_1} \propto \frac{1}{\rho^2 v^2} \left(\frac{V^2}{\hbar^2} \right) \left(\frac{kT}{\hbar} \right)^3 \quad (2)$$

where ρ is the silicon density, v is the sound velocity, V is the parameter of the electron-phonon interaction, which in our case is proportional to $\Delta_0 \Delta^2$ with Δ describing separation of states caused by magnetic field or strains and the parameters of the SO coupling $\Delta_0 \approx 1 \cdot 10^{-6}$ meV for Li donor, which are in agreement with those describing the experimental g-factors measured in [3].

In the same time the LiO donor with orbital nondegenerate ground state, for which the Orbach process [1] with relaxation rate $\tau^{-1} \propto e^{-\Delta/kT}$ is important. Note also, that $\Delta_0 \approx 1.5 \cdot 10^{-2}$ meV as well as other measured parameters for LiO complexes are in good agreement with those obtained from optical spectra [5]. W-band measurements show that Li spectrum can be observed at higher temperature (15 K) which caused by low spin-relaxation rate at high magnetic field. Therefore one can suggest that strains are less important even for X-band measurements. Comparing the SO coupling parameters for Li and LiO centers one can conclude that for lithium complexes the SO contribution comes not from lithium but from another component of the defect (oxygen in that case).

Summary

We studied spin relaxation times for Li donors in monoisotopic ^{28}Si over the temperature range 4–20 K. Comparison of the obtained spin-lattice relaxation times for the states of the isolated donor center and lithium complex LiO showed that due to the presence of orbital degeneracy, relaxation is faster for isolated lithium than the complexes LiO, for which the ground state is not degenerate. For the lithium donor the relaxation is well described by Blume-Orbach process, whereas the Orbach process is dominant in the spin relaxation of the LiO center. Investigations of the spin relaxation rates also allowed us to measure parameters of the spin-orbit coupling, which are $\sim 1 \cdot 10^{-6}$ meV and $\sim 1.5 \cdot 10^{-2}$ meV for isolated Li center and the LiO complex, respectively.

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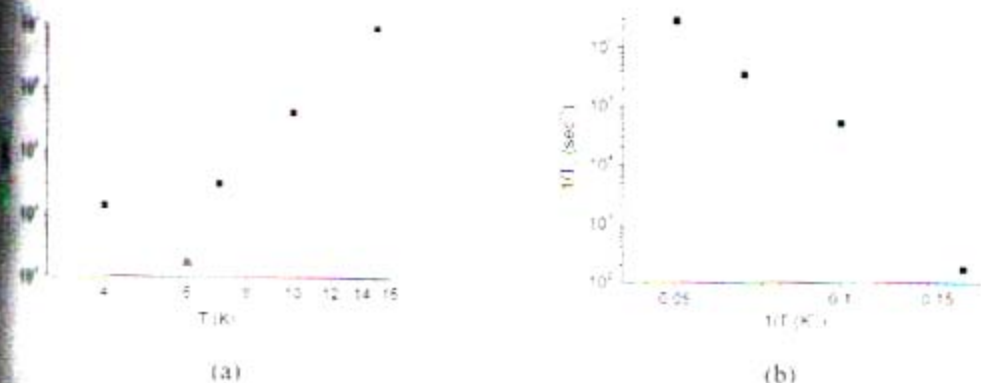


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