Lande factor of the conduction electrons in silicon: temperature dependence

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Abstract. Temperature dependence of the electron g-factor in silicon has been investigated both theoretically and experimentally. Theoretical consideration is based on the renormalization of the electron energy in a weak magnetic field by the electron-phonon interaction in the second-order perturbation theory. Interaction of the electron subsystem with the lattice vibrations results in decreasing the conduction electron g-factor. This decreasing was observed experimentally in the electron spin resonance studies for n-Si samples.

1. Introduction

Since pioneer demonstration of the spin injection and detection in Si [1], silicon becomes a perspective material for spintronics due to weak spin-orbit interaction, long spin relaxation time and large spin diffusion length in comparision with typical III-V semiconductors such as gallium arsenide. One of the most important characteristics of conduction electrons in various systems with spin-orbit coupling is the spin relaxation rate. Spin relaxation in silicon mainly occurs through the Elliott [2] and Yafet [3] mechanism, where the spin flip processes are caused by electron-phonon interaction. Quantitative theoretical studies of the Elliott-Yafet spin relaxation in silicon [4] yields the spin relaxation rate proportional to a third power of temperature \( T \). This is in good agreement with the experimental data. The spin relaxation rate can be extracted from the line width of the conduction electron spin resonance (CESR).

Another important characteristic of conduction electrons in magnetic field is their Lande g-factor, which is characterized by the position of the CESR line. First experimental investigations of the conduction electron g-factor were carried out by Wilson and Feher [5]. The measured value for “free” carriers was found to be \( g = 1.99875 \pm 0.0001 \). In silicon each conduction valley has an axial symmetry, so the g-factor becomes a tensor with two, longitudinal \( g_{||} \) and transverse \( g_{\perp} \), principal values. The measured value \( g \) is isotropic due to cubic symmetry of the Brillouin zone and has the average form over all six conduction band valleys:

\[
g = \frac{1}{3} g_{||} + \frac{2}{3} g_{\perp}.
\]  

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In contrast to the spin relaxation rate, there is no information in literature about the temperature dependence of the electron g-factor in silicon. So, in this work we first theoretically discuss and experimentally demonstrate this temperature dependence.

2. Experimental results
We studied the electron g-factor in CESR spectra measurements. We have observed dependence of g-factor of conduction electrons in silicon as a function of temperature and found that in temperature range 80 - 250K they are alike for different donors and their concentrations. The measurements are performed on the spectrometer “Bruker EMX 10/12” using helium cryostat with a system of a temperature control (3.8-300 K) “ER 4112 HV”. We use natural silicon samples doped with lithium and phosphorus to make some concentration of electrons in the conduction band. Donor concentrations in both samples were very close to minimize difference in the spin flip process intensity.

![Figure 1. Calculated (solid line), and measured (dots and circles) temperature dependences of the average electron g-factor in Si sample doped with phosphorus (red dots) and lithium (blue circles). Phosphorus and lithium concentrations are $3.7 \times 10^{18}$ cm$^{-3}$ and $3.3 \times 10^{18}$ cm$^{-3}$, respectively. Calculations were carried out in accordance with Eq. (9). The phonon energy $\hbar \omega$ in Eq. (9) was taken to be 10 meV.](image)

The experimental results are presented in figure 1. As temperature increases from zero to ~80 K, a monotonous rise of the g-factor value takes place. In this temperature range electrons still localized on the donor centres and have the discrete energy spectra, so it can occupy the singlet $A_1$ or the triplet $T_2$ and doublet $E$ states. Each of these states can be described by different g-factors, and changing the electron distribution among these states with temperature rising can leads to rising g-factor. Consideration of this effect in more details goes beyond the scope of the present paper. However at higher temperatures the donors become ionized and the electrons can propagate over the sample. In this temperature range one can see approximately linear decrease of the g-factor, which can be explained by the modulation of the lattice spin-orbit interaction by phonons. Below, we discuss some theoretical approach to this problem.

3. Theoretical model
Theoretical study of the g-factor temperature dependence is based on the renormalization of the electron energy in the external magnetic field by the electron-phonon interaction. Within the framework of a many-body picture the renormalization of the excitation energies by lattice vibrations can be defined by the equation [6]

$$\varepsilon(k) = \varepsilon^{(0)}(k) + \text{Re} \sum' \varepsilon(k),$$

where $\varepsilon^{(0)}(k)$ and $\varepsilon(k)$ are unperturbed and renormalized electron energies, respectively, and $\text{Re} \sum' \varepsilon(k)$ is the self-energy real part that can be presented in covalent semiconductors, such as silicon, using the Rayleigh-Schrödinger perturbation theory [7]:
\[ \text{Re} \sum' (\varepsilon, k) = \sum_{q \neq q} \left( n_{qk} + \frac{1}{2} \right) \frac{|V(q)|^2}{\varepsilon^{(0)}(k) - \varepsilon^{(0)}(k \pm q) \pm \hbar \omega_\lambda(q)}. \]  

where \( V(q) \) is the matrix element describing the electron scattering (from the state \( |k\rangle \) to the \( |k \pm q\rangle \) state) accompanied by absorption (upper sign) or emission (lower sign) of a phonon with the wave vector \( q \) and polarization \( \lambda \), \( \omega_\lambda(q) \) and \( n_{qk} \) are the frequency and the occupation number of phonons. In what follows, we replace the phonon occupation numbers by their equilibrium values describing the Bose-Einstein statistics.

If the spin-orbit interaction is taken into account, the electron states become the states with an effective generalized spin that differs from the standard spin moment. We will denote these states as effective spin-up \( \uparrow \) or spin-down \( \downarrow \) vectors. In the absence of magnetic field the spin-up and spin-down states have the same energies (the Kramers degeneracy). In the external magnetic field \( \mathbf{H} \) oriented along one of the valleys the electron energy has the additional Zeeman term \( \sigma \mu_0 g_i H/2 \), where \( \mu_0 \) is the Bohr magneton, \( g_i \) is the g-tensor principal value, \( i = \perp, \parallel \) for transverse and longitudinal components, respectively, and \( \sigma = \pm 1/2 \) are the effective-spin projections on the magnetic field. In that case the Zeeman term is also renormalized, and the total electron energy has the form

\[ \varepsilon(k) + \sigma \mu_0 g_i H = \varepsilon^{(0)}(k) + \sigma \mu_0 g_i^{(0)} H + \sum_{q \neq q} \left( n_{qk} + 1/2 \right) \frac{|V^{(i)}(q)|^2}{\varepsilon^{(0)}(k) - \varepsilon^{(0)}(k \pm q) - \hbar \omega_\lambda(q)}. \]  

where \( g_i^{(0)} \) and \( g_i \) are unperturbed and renormalized principal values of the g-tensor, respectively, \( V^{(i)}(q) \) is the spin-dependent momentum scattering matrix element for the electron in the \( i \)-th valley. Thus, if scattering conserves the spin, only the translatory-motion energy is modified. On the contrary, spin-flip processes modify the Zeeman energy. Using standard approach \( \mu_0 g_i H \ll \varepsilon(k) \), and neglecting the phonon-absorption process, whose contribution seems to be less compared to the phonon-emission process, one can obtain

\[ g_i = g_i^{(0)} - 2g_i^{(0)} \sum_{q \neq q} \frac{(n_{qk} + 1)|V^{(i)}(q)|^2}{\varepsilon^{(0)}(k) - \varepsilon^{(0)}(k \pm q) - \hbar \omega_\lambda(q)} \]  

Here, \( V^{(i)}(q) \) is the spin flip matrix element which can be written as [3,8]

\[ |V^{(i)}(q)| = A_i q^2 \sqrt{\hbar/2 \rho V \omega_\lambda(q)}, \]

where \( \rho \) and \( V \) are the silicon density and the sample volume, respectively, \( A_i \) are some constants symbolically referred to as spin deformation potentials.

Considering the zero-temperature limit we should set \( n_{qk} = 0 \) in Eq. (5). In this case Eq. (5) yields the zero-temperature renormalization of the g-factor by emitting and subsequent absorbing virtual phonon. Evidently, measured low-temperature conduction electron g-factor, such as Wilson and Feher’s \( g = 1.9987 \), includes this correction. Consequently, we will use the low-temperature experimental values as zeroth approximation:

\[ g_i(0) = g_i^{(0)} - \frac{\hbar A_i^2 g_i^{(0)}}{\rho V} \sum_{q \neq q} \frac{q^4}{\omega_\lambda(q)(\varepsilon^{(0)}(k) - \varepsilon^{(0)}(k - q) - \hbar \omega_\lambda(q))}. \]  

while \( T \)-dependent correction \( \delta g_i(T) \) will be defined by
The main contribution to the sum over \( q \) in Eq. (8) comes from the intervalley phonons connecting different valleys in the electron Brillouin zone. Taking these contributions into account, and averaging over acoustic phonon modes and electron valleys, it is possible to obtain the following estimation for the \( T \)-dependent correction:

\[
\delta g(T) = \frac{-hA^2}{\rho \omega} \sum_{q} n_{q} q^4 \omega_{q} (\varepsilon^{(0)}(q) - \varepsilon^{(0)}(k - q) - h\omega_{q}(q))^2.
\]

(8)

where \( q_{0} \) is a typical wavevector of the intervalley phonon, and \( \omega = \omega(q_{0}) \) is average phonon frequency corresponding to the phonon energy \( h\omega \) whose value may be estimated as 10 – 20 meV. The calculated dependence \( \delta g(T) \) is presented in figure 1 along with the experimental data. It is seen that the theoretical estimations agree (at least qualitatively) with the measured values. However, to achieve the quantitative agreement, more rigorous calculations are necessary. In particular, theory should answer the following question: how the donor type influences the Zeeman splitting if the donors are ionized, and the electrons become, in fact, free. Presumably, the spin-orbit interaction and, consequently, the spin-dependent momentum scattering matrix element \( V_{\sigma\sigma'}(q) \) depend on the donor type. This dependence has to be taken into account to explain different experimentally observed values of the electron \( g \)-factor in Si doped with different donors. So far, within the framework of the suggested theoretical treatment, no any specific features of various donors have been considered.

4. Conclusion

Generally speaking, modification of the \( g \)-factor is caused by virtual phonon-induced spin flip processes occurring between the initial, intermediate, and final electron states, where the final and initial states completely coincide. This, presumably, implies that the Elliott-Yafet mechanism of the spin relaxation is the main one for the considered system.

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