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On the anomalous muonium hyperfine field in silicon

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Abstract

The muon spin precession in the axial-symmetric muonium Mu_{bc} was studied in a magnetic field applied along the initial muon polarization which was, in turn, parallel to the [111] axis of a silicon single crystal. Hyperfine fields were measured at temperature $T = 12$ K. The transversal parameter $A_\perp = 92.58(2)$ MHz is in good agreement with work by Blazey *et al* 1983 *Phys. Rev.* B **27** 15, but $A_\parallel = 16.52(6)$ MHz obtained in this work is less than the value published by Blazey *et al* by 0.29 MHz. This discrepancy is attributed to the accuracy of determination of the angle between the [111] axis and the magnetic field direction.

Positive muons implanted inside a silicon crystal can form two types of muonium: isotropic Mu_t at a tetragonal site and anisotropic muonium at a bond-centred site Mu_{bc} [1]. As the temperature is raised Mu_{bc} ionizes [1, 2], but at low temperature it is a stable and immovable particle on the timescale of the muon lifetime. As a consequence of its location Mu_{bc} has a very anisotropic hyperfine interaction that is characterized by two parameters $A_\perp$ and $A_\parallel$. Experimental values of parameters $A_\perp = 92.59(5)$ MHz and $A_\parallel = 16.79(1)$ MHz were obtained in the work [1, 2].

The Mu_{bc} hyperfine fields, which are directed along lattice diagonals, do not necessarily coincide with the direction of the applied external field. When the external field B is directed along the z-axis, the time evolution of the muon spin in Mu_{bc} is described by the axial-symmetric spin Hamiltonian [3]

$$H = g_e\mu_e B S_z - g_m\mu_m B I_z + A_\parallel S_z I_z + 1/2 A_\perp(S_+ I_- + S_- I_+) \qquad (1)$$

where $g\mu = \gamma$ denotes the gyromagnetic ratio of electron (e) and muon (m) and I and S represent the spins of the muon and electron, respectively. In the work [3] the hyperfine parameters $A_\perp$ and $A_\parallel$ were obtained from the sum and the difference between the two mSR frequencies at transverse magnetic field. This method does not require precise measurements of an external magnetic field, but the angle between the [111] axis and the field must be precisely determined. In high magnetic fields, one can ignore the influence of the muon magnetic moment on the electron. In this case the states with the electron spin parallel and antiparallel to the field are practically decoupled and the spin dynamics can be described [4] by the two effective Hamiltonian operator, which provides the following relation [5] for the muon spin precession frequency ω:

$$(\omega/\gamma_\mu)^2 = (B - B_\nu)^2 + \cos^2\theta[B_\nu^2 + 2BB_\delta - 2B_\nu B_\delta] \qquad (2)$$

where θ is the angle between the symmetry axis of $\mathrm{Mu_{bc}}$ and the external field B. Hyperfine fields are bounded with appropriate parameters $B_\nu = -hA_\perp/2\gamma_\mu$ and $B_\delta = h(A_\parallel - A_\perp)/2\gamma_\mu$, $\gamma_\mu = g_\mathrm{m}\mu_\mathrm{m} = 13.5534$ MHz kOe^{-1}.

Expression (2) can be used to analyse the field and angle dependence of the muon precession frequencies. It is easy to see that the precession frequency has a minimum at $B \cong 3.1$ kOe and the angle dependence disappears in the field $B \cong 2$ kOe. By measuring the frequency $\omega(B)$, the determination accuracy of the transversal constant is directly defined by the magnetic field, but the accuracy of the longitudinal constant $A_\parallel$ depends substantially on the θ angle. The analysis of the measurement method [3] (see (2) in this work) also shows that at $B = 1$ kOe used in [3] $A_\parallel$ is much more sensitive to θ than $A_\perp$.

In the present work we observed the muon spin precession in the $\mathrm{Mu_{bc}}$ state in longitudinal fields (B is parallel to initial muon polarization) and determined the hyperfine interaction parameters from the magnetic dependence of the precession frequency. Measurements were carried out at PSI (Switzerland) on the GPD set-up. The sample was a disc cut from a high-purity silicon single crystal. The disc diameter was 33 mm, the thickness—5 mm. Neutron diffraction measurements show that the disc axis was directed along the crystallographic axis [111] with an accuracy of 1°. A longitudinal magnetic field was applied along the [111] crystal axis. Such a geometry enabled us to see the muon spin precession at the temperature $T = 12$ K and to measure the longitudinal field dependence of this frequency. The muon spin relaxation rate was found to be small ($\lambda < 0.01\ \mu\mathrm{s}^{-1}$) below 100 K. This fact may be considered as evidence of the low carrier concentration $n < 5 \times 10^{12}\ \mathrm{cm}^{-3}$ and explained by the absence of any visible $\mathrm{Mu_{bc}}$ kinetics [1]. The experimental time dependence of the muon polarization $P(t)$ at the temperature 12 K in the longitudinal field $B = 3.1$ kOe is shown in figure 1. One can see clear oscillations of the muon spin precession related to axial-symmetric muonium. The rather irregular behaviour of the oscillation amplitude is explained by the presence of several frequencies. The appropriate Fourier spectrum, shown in the figure 1 inset, has three distinct peaks. Three frequencies correspond to three muonium positions where $\mathrm{Mu_{bc}}$ states are located. As a result of a small deviation of the [111] axis from the external field direction the symmetry axes of $\mathrm{Mu_{bc}}$ states have different angle θ to the B direction and correspondingly different field values.

Figure 2 shows the experimental longitudinal field dependence of precession frequencies in the field region 2.0–4 kOe. Frequency values were obtained by fitting of the mSR time spectra using three frequencies as free parameters. Relative errors of frequencies $\Delta f/f$ were less than $\pm 2 \times 10^{-4}$. Hyperfine constants and the angles θ_i were calculated using the dependences shown in figure 2 by comparison of Hamiltonian parameters (1) and experimental curves $\omega_i(B)$. The values of ω were found by solving Schroedinger equation $H\psi = E\psi$ at a given magnetic field value for arbitrary fixed values of hyperfine constants with three θ_{io} angles. The standard least squares fit using numerical calculation of derivatives and the usual χ^2 criterion was performed after that. For small deviation of the magnetic field direction from the [111] axis (at the 10^{-4} level) the relation $\Sigma\cos\theta_i = 1$ is valid.

Results of calculation are shown in table 1, approximate $\omega_i(B)$ curves in figure 2.

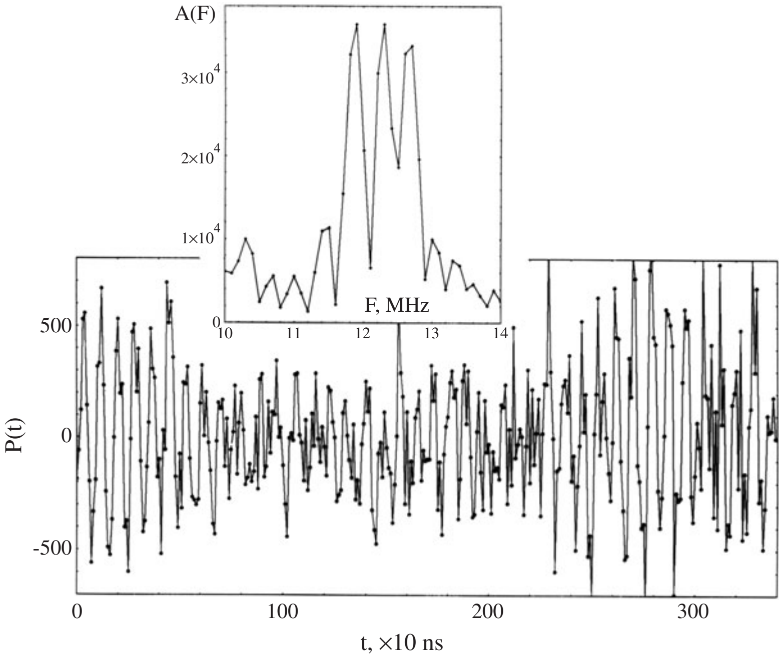

Figure 1. The time dependence of the muon polarization in the magnetic field $B = 3.1$ kOe at $T = 12$ K in silicon. The channel width is 10 ns. The inset shows the precession Fourier spectrum for the $\mathrm{Mu_{bc}}$ state. Frequency values were defined according to the harmonic N number using the relation $F = N \times 0.0499$ MHz.

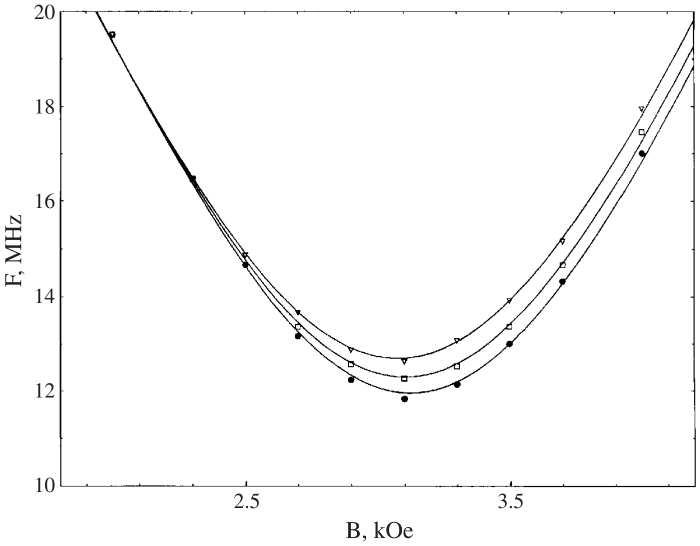

Figure 2. Field dependences of muon precession frequencies in silicon at $T = 12$ K. The three curves correspond (from the top down) to axis slope angles $\theta_i = 69.80°$, 70.63° and 71.16°.

The calculated value of $A_\perp$ is in good agreement with experimental data [3], but the longitudinal component value $A_\parallel$ is less by 1.8%, far beyond one standard deviation. This

Table 1. Measured hyperfine interaction parameters $A_\perp$ and $A_\parallel$ and the angle between the [111] axis and the external field θ_i.

$A_\perp$ (MHz)	$A_\parallel$ (MHz)	θ_i	References
92.59(5)	16.819(11)	—	[3]
92.58(2)	16.52(6)	69.80(1) 70.63(1) 71.16(1)	This work

discrepancy may be caused by the uncertainty in θ_i, because $A_\parallel$ is more sensitive to θ_i than the $A_\perp$ value. In our experiment the [111] axis angles values were obtained as a best fit parameter. This fact enables one to determine angle values with a high accuracy. The method of angle determination described in [1, 2] is more difficult in application.

It should be noted in conclusion that the multi-frequency character of the spectrum can be used to adjust the crystal orientation *in situ*. The precision of such an adjustment, determined or limited by the width of a precession frequency, can reach 0.1°.

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