

Muonium dynamics as a probe for depth-resolved properties of 4H-SiC

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This study establishes a baseline for muonium (Mu) charge-exchange dynamics in n-type 4H-SiC through a detailed low-energy muon spin rotation (LE- μ SR) investigation. Epitaxially grown and ion-implanted samples with nitrogen and phosphorus donors were characterized to assess the effect of carrier concentration and doping method on defect formation. LE- μ SR enabled nanometer-scale depth profiling of near-surface and implanted regions, revealing variations in charge carrier concentration due to fixed surface charges. The temperature dependence of the diamagnetic fraction and phase provided direct evidence of the Mu^0 to Mu^- transition, with extracted activation energies consistent with known donor ionization energies. Additionally, high-field μ SR was used to analyze the Mu dynamics, and Monte Carlo simulations were used to model the Mu^0 electron capture process. The simulation results offer a quantitative method to extract free electron concentrations from LE- μ SR data, enhancing its capability to characterize the activation of dopants and carrier depth profiles. We demonstrate that LE- μ SR is a powerful depth-resolved tool that can provide insights for optimizing the fabrication of reliable SiC devices for power electronics.

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I. INTRODUCTION

Silicon carbide (4H-SiC) is a wide-bandgap semiconductor that is increasingly adopted due to its suitability for high-temperature, high-power, and high-frequency applications. One of the key technological developments allowing the manufacturing of reliable devices is the epitaxial growth of 4H-SiC, which enables the formation of layers with precise control over their thickness, doping concentrations, and relatively low defect densities [1,2]. Selective doping is another essential step in device manufacturing. However, due to the strong silicon-carbon (Si—C) bonds in the crystal lattice, the dopant diffusivity is very low. As a result, ion implantation is the preferred method for introducing dopants into specific regions of the semiconductor material. While this technique allows for accurate control over doping profiles, it also introduces significant lattice damage that must be carefully

managed [3]. For n-type doping, nitrogen (N) and phosphorus (P) are commonly used, while p-type doping is typically achieved using aluminum (Al), and less frequently, boron (B) [4,5].

A postimplantation annealing (PIA) step is required to recover the structure and electrically activate the dopants by promoting their inclusion into the SiC lattice. Annealing between 1600 °C and 1700 °C results in almost 100% electrical activation of N and P donors [4,6]. During the high-temperature annealing, the samples are usually coated with a carbon (C) cap to prevent Si desorption and surface degradation [7,8]. The presence of a C-cap allows carbon to be injected into SiC, contributing to the reduction of the density of carbon vacancies (V_C) [9] and the formation of other carbon-related defects [10,11].

Deep-level transient spectroscopy (DLTS) is commonly used in the study of defects in the bulk of semiconductors, since electrically active defects and their location within the bandgap can be identified. DLTS measurements have shown that even after PIA, some of the defects created during ion implantation are still present and can extend beyond the projected implantation profiles [12]. However, the DLTS probing depth and sensitivity to defect densities are limited by the doping concentration, and it is hard to obtain information about the near-surface region (top hundred nanometers). Therefore, low-energy muon spin

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rotation spectroscopy (LE- μ SR) [13–15] was used to study the effect of N and P ion implantation by directly probing the implanted regions from the surface to a depth of 150 nm, while varying the muons' implantation energy. LE- μ SR studies of 4H-SiC have allowed meaningful insight into the properties of defects that affect the reliability of devices (V_C) and ones with applications in quantum technologies (V_{Si}) [16,17]. Oxide-semiconductor systems were investigated, and the effects of oxidation and postannealing on the creation and passivation of defects created on the interface and near-interface could be determined [18–20]. The muon is also very sensitive to the charge carriers in its vicinity [21] and has been used to quantify changes in the electrical environment as a function of depth with nanometer depth resolution [22,23].

We present the high-field μ SR measurements performed using the high-field and low temperature instrument (HAL-9500), where the temperature dependence of the μ SR signal is used to characterize the different muonium (Mu) states formed in SiC and transitions between them. A good understanding of the Mu dynamics in the material, e.g., activation energy of the transition, lattice sites and charge states occupied, is crucial to use the muon as a probe for the processing-induced defects.

Previous μ SR works [24,25] show the presence of two distinct Mu^0 centers in the high-field regime ($B > 0.5$ T) with hyperfine constants $A_{HF} = 3030$ MHz and 2825 MHz, called Mu_1 and Mu_2 , respectively. These states are observed in n-type, p-type and high resistivity 4H-SiC. However, important details about the samples studied with μ SR, e.g., doping concentration, growth process, were not reported. More recently, LE- μ SR measurements at low magnetic field reveal a previously unreported weak anisotropy of the hyperfine coupling [18]. This is seen as a splitting in the Mu^0 precession frequency into two lines, which stays constant in the measured field range.

The sensitivity of the muon probe to defects and charge carrier density, combined with its nanometer depth resolution, means that LE- μ SR can provide information about the activation of donors in n-type 4H-SiC and reveal differences between the doping process during epitaxial growth and ion implantation, as well as the different

defects created due to N- vs P-implantation. By using LE- μ SR, the implantation region and the near-surface are directly investigated. This investigation is a significant building block in the characterization of 4H-SiC interfaces and devices, providing a baseline of the LE- μ SR sensitivity to the charge carrier concentration.

II. METHODOLOGY

A. Sample preparation

For this study, n-type 4H-SiC epilayers with a thickness of 10 μ m grown on highly doped 4H-SiC substrates were characterized with LE- μ SR. The epilayer is a high-purity single crystal, grown on substrates that are 4° off the (0001) c axis, maintaining the 4H stacking sequence. The details on sample preparation are found in Table I. The epitaxial samples were doped with nitrogen during growth and have doping concentrations of $4 \times 10^{15} \text{ cm}^{-3}$ and $1 \times 10^{17} \text{ cm}^{-3}$. The implanted samples were prepared on n-type epilayers with $N_D = 3 \times 10^{15} \text{ cm}^{-3}$ background doping. In order to create regions with well-defined doping concentration with thicknesses between 250 and 350 nm, multiple ion (N or P) implants at different energies and fluences were performed at the Fraunhofer IISB in Erlangen, Germany. The resulting implantation box profiles are shown in Fig. 1. The N-implantation consisted of five implantation steps performed with energies between 200 and 400 keV, and the P-implantation of six steps with energies between 300 and 800 keV. The total fluence of the implantation is $4 \times 10^{12} \text{ cm}^{-2}$ and $4 \times 10^{13} \text{ cm}^{-2}$ for the doping concentrations $2 \times 10^{17} \text{ cm}^{-3}$ and $1 \times 10^{18} \text{ cm}^{-3}$, respectively. Before implantation, 550 nm of SiO_2 was deposited using plasma-enhanced physical vapor deposition (PECVD). The sacrificial SiO_2 layer is used to guarantee the implantation peaks of the ions are in the SiC epilayer. Implantation was performed with the samples held at approximately 500°C to increase dynamic annealing of the lattice damage simultaneously with the formation of ion damage [26]. After implantation, the deposited oxide was removed using hydrofluoric (HF) acid. Finally, the samples were cleaned and coated with a carbon cap (C-cap), to be annealed at 1650°C for 30 min.

TABLE I. Description of the 4H-SiC samples investigated with LE- μ SR. The parameters are the doping concentration N_D , donor species, doping process, and PIA with a carbon capping layer. Implantation was performed to form the box profiles shown in Fig. 1. N_D was extracted from capacitance-voltage measurements.

Sample name	N_D (cm^{-3})	Donor species	Doping process	PIA parameters
Epi-N15	4×10^{15}	Nitrogen	Epitaxial growth	...
Epi-N17	1×10^{17}	Nitrogen	Epitaxial growth	...
Imp-N17	2×10^{17}	Nitrogen	Ion implantation	30 min at 1650°C
Imp-N18	1×10^{18}	Nitrogen	Ion implantation	30 min at 1650°C
Imp-P17	2×10^{17}	Phosphorus	Ion implantation	30 min at 1650°C
Imp-P18	1×10^{18}	Phosphorus	Ion implantation	30 min at 1650°C

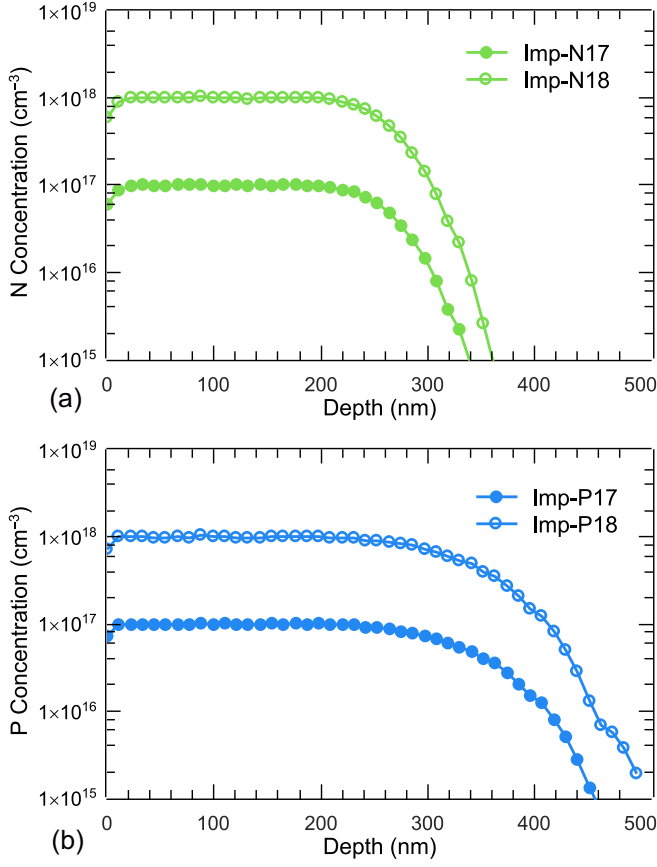


FIG. 1. Box profiles for the implantation of (a) N^+ and (b) P^+ ions in the 4H-SiC epilayer samples. The ion-implantation profiles were obtained with SRIM simulations [27,28].

After annealing, the carbon cap was removed using an oxygen plasma, and subsequently cleaned in HF.

An additional n-type 4H-SiC sample (N-doped), with a 150 μm thick epilayer with $N_D = 2 \times 10^{14} \text{ cm}^{-3}$ grown on a 350 μm substrate and purchased from Ascatron, was investigated in the HAL-9500 instrument, which uses a conventional 4.1 MeV surface muon beam to study the bulk of the material.

B. Muon spin spectroscopy

The muon spin rotation technique (μSR) uses the positive muon μ^+ as a local probe to study the electrical and magnetic properties in solids [29–32]. A beam of nearly 100% spin-polarized muons is implanted into the sample under study. The implanted μ^+ decays with a mean lifetime of $\tau_\mu \approx 2.2 \mu\text{s}$ and spontaneously emits a positron preferentially in the direction of the muon spin at the time of the decay.

By detecting the emitted positron, the time evolution of the muon spin polarization in the sample is obtained. In the sample, the muon comes to rest at an interstitial site of the host lattice and can be treated as a light isotope of hydrogen called muonium (Mu). In semiconductors and

insulators, the μ^+ probe can stay positive in the Mu^+ state, capture an electron and form the paramagnetic state Mu^0 , or capture even two electrons to form the negative Mu^- state, if enough electrons are available in its surroundings. The charged states Mu^+ and Mu^- without coupling to an unpaired electron are called diamagnetic. In the measurements, we used a transverse-field configuration (TF- μSR), where an external magnetic field was applied perpendicular to the spin of the incoming muon, inducing precession of the muon spin. In the case of the two diamagnetic Mu states, the muon spin precesses at its Larmor frequency, whereas the hyperfine coupling with the unpaired electron in the Mu^0 state causes different muon spin precession frequencies, which are typically very distinct from the Larmor frequency [21]. The muon spin precession frequencies corresponding to the transitions between the four hyperfine levels of the Mu^0 state can be detected, and information about the occupancy and dynamics of the diamagnetic and paramagnetic states can be extracted.

Typically, μ^+ beams with an energy of 4.1 MeV are available at proton accelerator facilities. At this energy, the muons penetrate several hundred micrometers deep and the bulk of the material is probed. We performed high-field μSR measurements in HAL-9500 under a high magnetic field of 6 T to identify the TF precession frequencies of the muonium states in low-doped 4H-SiC and to compare with previous μSR experiments [24]. To stop the incoming muon beam in the low-doped 150 μm epilayer, the muons were slowed down by using a degrader. The degrader was chosen by simulating the stopping of the muons with SRIM [27,28] (Fig. 2) and consisted of a stack of 200 μm Al, 10 μm Ag, and 25 μm Al.

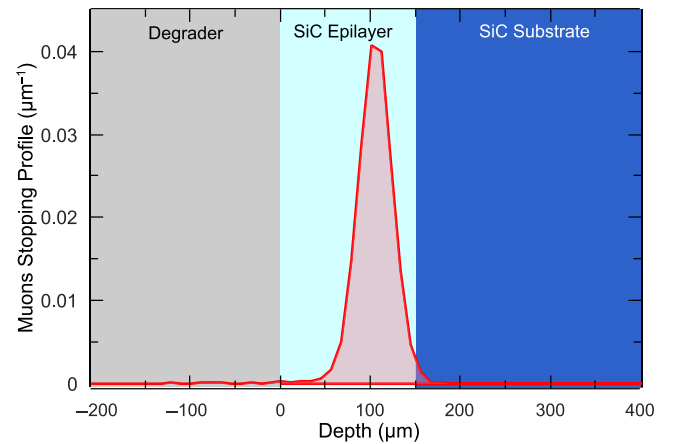


FIG. 2. Stopping distribution of the muon beam calculated with SRIM simulation [27,28]. The curve shows that the majority of the muons stop in the 150 μm thick SiC epilayer, with a small fraction of the muons stopping in the highly doped substrate layer.

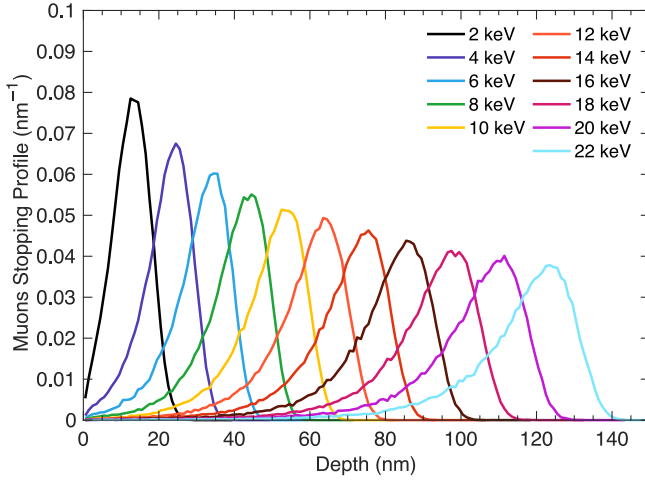


FIG. 3. Stopping profiles of muons for the different implantation energies, obtained for 4H-SiC with the Monte Carlo simulation program TRIM.SP [33,34].

C. Low-energy μ SR

LE- μ SR is an extension of μ SR with interesting applications in the study of thin films, surfaces, and interfaces, due to its nanometer depth resolution. The probing depth can be varied from the near-surface region to approximately 150 nm in 4H-SiC [13,14]. The stopping profiles of the muon beam for different implantation energies are shown in Fig. 3 and are simulated using the Monte Carlo simulation program TRIM.SP [33,34].

The LE- μ SR measurements were performed at TF values of 0.7 and 10 mT. It is necessary to collect data at low magnetic fields ($B < 1$ mT) to observe the muonium precession frequency, due to the upper detection limit of about 60 MHz of the low-energy muon spectrometer (LEM), which stems from the limited time resolution of

LEM of about 5 ns. At 0.7 mT, the diamagnetic and the Mu_1 paramagnetic components can be spectroscopically detected, whilst the Mu_2 paramagnetic component depolarizes too quickly to be observed. At this low field, the transition frequencies between the triplet states in Mu^0 with isotropic hyperfine coupling ν_{12} and ν_{23} overlap, resulting in a single Mu^0 precession frequency. However, a splitting of this precession frequency, due to a weak anisotropy of the hyperfine coupling [18,24], results in the spectrum shown in Fig. 5(a). At 10 mT, the Mu^0 transition frequencies are higher than the maximum resolution of the LEM spectrometer, thus only the diamagnetic component is observed and analyzed.

The temperature dependence was measured in HAL-9500 and LEM between 10 and 310 K to observe the temperature-activated transitions of the Mu states before and after the charge carriers were free in 4H-SiC. The energy dependence was measured in LEM at 260 K, when the activation of the donors is approximately 100%, to probe changes with depth in the epilayer and implanted region. The muon implantation energy was varied between 2 and 22 keV, corresponding to a mean probing range of 5 and 130 nm (Fig. 3), respectively.

D. Data analysis

The μ SR data analysis was performed using the *musrfit* software [35]. In HAL-9500, at a transverse magnetic field of 6 T, five lines are observed in the Fourier spectrum [see Fig. 4(a)]—one diamagnetic line and four lines resulting from the formation of two different muonium configurations in 4H-SiC (Mu_1 and Mu_2). At 6 T, two precession frequencies are observed for each Mu state, ν_{12} and ν_{34} . The data obtained from HAL-9500 were thus fitted with five components as follows:

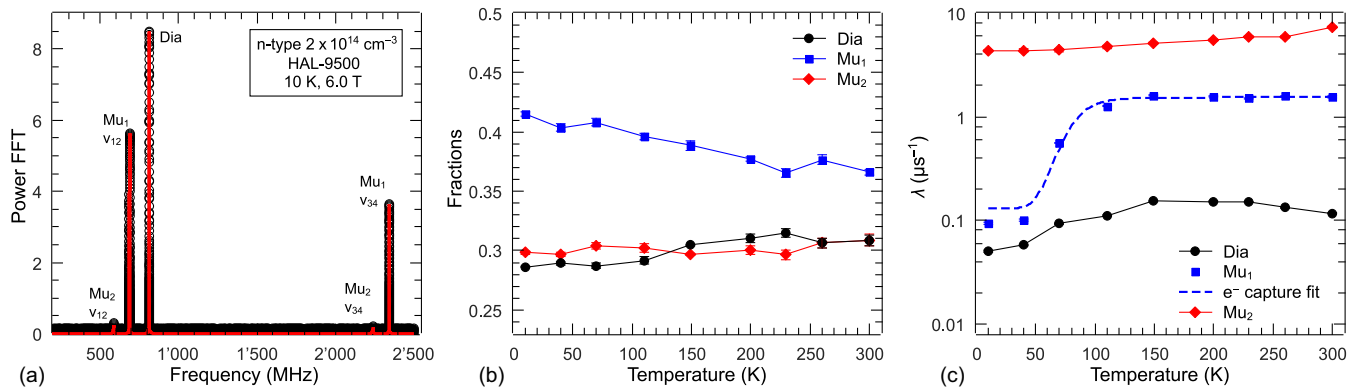


FIG. 4. (a) Fourier transform power spectrum of the time spectrum collected in HAL-9500. The Mu_1 and Mu_2 states, with distinct hyperfine coupling frequencies, are observed in addition to the diamagnetic line in the bulk of thick epilayer at 10 K and 6 T. Results from HAL-9500 measurements in n-type ($2 \times 10^{14} \text{ cm}^{-3}$, N-doped) 4H-SiC with an applied magnetic field of 6 T. Temperature dependence of (b) the fractions of the diamagnetic (Dia) and paramagnetic Mu_1 and Mu_2 components, and (c) the corresponding relaxation rates λ . The solid lines in (b),(c) are guides to the eyes, and the dashed line is the fit curve using Eq. (A5) to model the Mu_1 electron capture process.

$$\begin{aligned}
A(t) = & A_D \cdot \exp(-\lambda_D \cdot t) \cdot \cos(2\pi\nu_D t + \phi_D) \\
& + A_{\nu_{12}}^{\text{Mu1}} \cdot \exp(-\lambda_{\nu_{12}}^{\text{Mu1}} \cdot t) \cdot \cos(2\pi\nu_{\nu_{12}}^{\text{Mu1}} t + \phi_{\nu_{12}}^{\text{Mu1}}) \\
& + A_{\nu_{34}}^{\text{Mu1}} \cdot \exp(-\lambda_{\nu_{34}}^{\text{Mu1}} \cdot t) \cdot \cos(2\pi\nu_{\nu_{34}}^{\text{Mu1}} t + \phi_{\nu_{34}}^{\text{Mu1}}) \\
& + A_{\nu_{12}}^{\text{Mu2}} \cdot \exp(-\lambda_{\nu_{12}}^{\text{Mu2}} \cdot t) \cdot \cos(2\pi\nu_{\nu_{12}}^{\text{Mu2}} t + \phi_{\nu_{12}}^{\text{Mu2}}) \\
& + A_{\nu_{34}}^{\text{Mu2}} \cdot \exp(-\lambda_{\nu_{34}}^{\text{Mu2}} \cdot t) \cdot \cos(2\pi\nu_{\nu_{34}}^{\text{Mu2}} t + \phi_{\nu_{34}}^{\text{Mu2}}).
\end{aligned} \quad (1)$$

The observed amplitude of the high-frequency lines is reduced due to the finite time resolution. Thus, all the amplitudes, including the A_g calibration, were corrected using the correction function $C(\nu)$ [36]:

$$C(\nu) = \exp[-(2\pi\nu\sigma)^2/2], \quad (2)$$

where the width is $\sigma = 66$ ps, calculated as

$$\sigma = \frac{1}{\pi\sqrt{2}} \cdot \sqrt{\ln \frac{A_{\nu_{12}}}{A_{\nu_{34}}} (\nu_{34}^2 - \nu_{12}^2)}. \quad (3)$$

Each component was fitted with its own relaxation rate λ . For each Mu^0 , $\lambda_{\nu_{12}}$ and $\lambda_{\nu_{34}}$ values are similar, thus the average λ_{Mu1} , and λ_{Mu2} were calculated.

The LE- μ SR time spectra in Fig. 5(a) were fitted with a three-component function of the form:

$$\begin{aligned}
A(t) = & A_D \cdot \exp(-\lambda_D \cdot t) \cdot \cos(2\pi\nu_D t + \phi_D) \\
& + A_{\text{Mu}} \cdot \exp(-\lambda_{\text{Mu}} \cdot t) \cdot [\cos(2\pi\nu_1 t + \phi_{\text{Mu}}) \\
& + \cos(2\pi\nu_2 t + \phi_{\text{Mu}})],
\end{aligned} \quad (4)$$

where A_D is the asymmetry of the diamagnetic component (either Mu^+ or Mu^-), λ_{Mu} is the exponential depolarization rate of Mu^0 , $\nu_{1/2} = \nu_{\text{Mu}} \pm \nu_a/2$ with the low-field muon spin precession frequency ν_{Mu} in the Mu^0 triplet state

without anisotropy, and $\nu_a = 1.7$ MHz is the small anisotropic component of the hyperfine coupling on top of the isotropic part of approximately 3000 MHz [18]. The phase ϕ_D of the diamagnetic signal is usually the angle offset of the decay positron detector in relation to the muon spin polarization at $t = 0$. However, a possible phase shift, observed as a function of temperature, indicates the occurrence of conversion between muonium states—due to a change of the muon spin precession frequencies [21]. The data collected at 10 mT were fitted using only the first component of Eq. (4), since only the diamagnetic contribution is observable in LEM at this field.

The asymmetry parameters A_D and A_{Mu} were converted to the corresponding fractions F_D and F_{Mu} by normalizing to the maximum asymmetry measurable in silver (A_{Ag}). The fractions are calculated as $F_D = A_D/A_{\text{Ag}}$ and $F_{\text{Mu}} = 2 \cdot A_{\text{Mu}}/A_{\text{Ag}}$. The factor of 2 in F_{Mu} accounts for the fact that only 50% of the Mu^0 polarization is observable in low fields [30].

Of note, deconvolution of the experimental data as a function of implantation energy and the stopping depth profile of the muon is performed to model the diamagnetic fraction as a function of sample depth, as detailed in Ref. [37]. The variation of F_D with depth using a multi-layer fitting approach allows observing local changes in carrier concentration, and to extract the charge carrier depth profiles.

E. Monte Carlo simulation of the electron capture

In semiconductors, transitions between the different muonium states may occur, depending on the temperature, concentration, and type of the free carriers present in the sample [21,23,38]. In n-type SiC, the electron capture process [39]

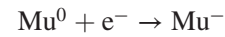
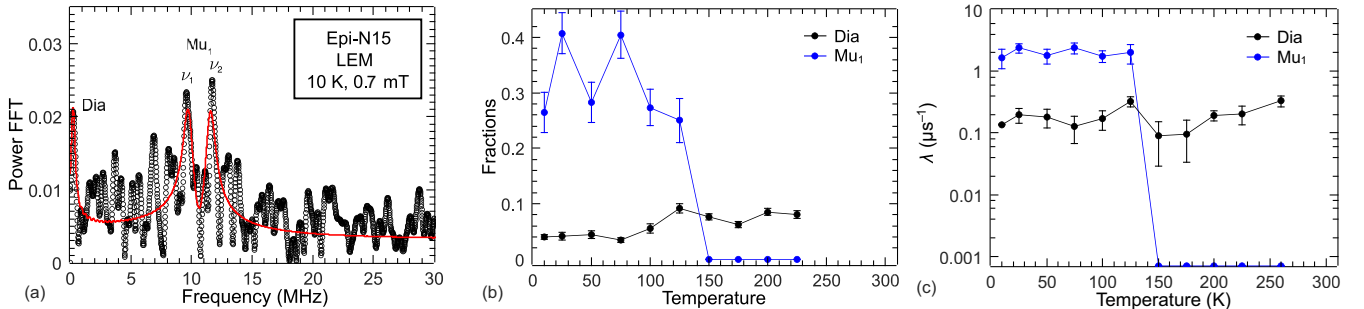


FIG. 5. (a) Fourier transform of the time spectrum collected in LEM. In the Epi-N15 sample, the diamagnetic and Mu_1 precession frequencies are observed at 10 K and 0.7 mT. The ν_{12} and ν_{23} transitions of the Mu^0 state are split into two lines, with frequencies $\nu_1 = 9.8$ MHz and $\nu_2 = 11.5$ MHz, respectively. LE- μ SR measurement in Epi-N15 of (b) the diamagnetic (Dia) and paramagnetic Mu_1 fractions and (c) the respective relaxation rates λ as a function of temperature, measured at 0.7 mT and an implantation energy of 19 keV. The Mu_1 relaxation rate becomes too high above 150 K, which leads to the disappearance of the Mu_1 precession lines. For simplicity, the Mu parameters were fixed at zero in this range.

occurs when the dopants are ionized ($T > 50$ K) [40] and is governed by the capture rate

$$\lambda_c = n \cdot v_e \cdot \sigma^{0/-}, \quad (5)$$

where n is the effective free electron concentration, v_e is the thermal velocity of the electrons, and $\sigma^{0/-}$ is the electron capture cross section for this process. Note that all these parameters are functions of temperature, as discussed in Appendix A.

The impact of the muonium dynamics in 4H-SiC was modeled using a Monte Carlo simulation [41,42] by calculating the temporal progression of the muon spin phase in a given magnetic field. In this work, only the electron capture process at 0.7 and 10 mT is considered. The information needed to generate TF- μ SR histograms is:

- (i) the fraction of implanted muons that exist in a neutral state Mu^0 at a time $t = 0$. It is assumed that $F_{\text{Mu}}(t = 0) = 0.95$, because at low temperatures a diamagnetic fraction of 0.05 is measured in 4H-SiC with LE- μ SR.
- (ii) the four precession frequencies ν_{ij} and respective probabilities a_{ij} for each simulated magnetic field. The transition frequencies used, and their probabilities, are shown for 0.7 and 10 mT in Table II.
- (iii) the rate of the capture process. The simulation was run for different λ_c in the range of 0.1 to 50 000 μs^{-1} .

The time t_c of the next electron capture event depends on λ_c and is "thrown" according to the probability distribution $\exp(-\lambda_c t)$. In the Mu^0 state, the muon spin precession is determined by the superposition of the precession frequencies ν_{ij} , weighted by their respective probabilities a_{ij} . If $t_c > t_d$, with t_d the muon decay time, the muon decays while still being in the Mu^0 state. If $t_c < t_d$, the electron capture process results in the final diamagnetic state Mu^- , and the muon spin continues to precess at its Larmor frequency at $t > t_c$ until it decays at t_d . More information on the Monte Carlo simulation methodology can be found in Refs. [41,42].

TABLE II. Transition frequencies ν_{ij} and probabilities a_{ij} of Mu^0 in 4H-SiC in an applied TF of 0.7 and 10 mT, assuming an isotropic hyperfine coupling constant $A_{\text{HF}} = 3030$ MHz, corresponding to the Mu_1 state in 4H-SiC.

Transition	0.7 mT		10 mT	
	ν_{ij} (MHz)	a_{ij}	ν_{ij} (MHz)	a_{ij}
ν_{12}	9.7	0.252	132.7	0.273
ν_{23}	9.8	0.248	145.8	0.227
ν_{34}	3020.2	0.252	2897.2	0.273
ν_{14}	3039.7	0.248	3175.7	0.227

III. RESULTS AND DISCUSSION

The high-field (6 T) measurements performed in HAL-9500 confirm the presence of the two Mu^0 configurations previously observed in 4H-SiC [24], as can be seen in Fig. 4(a).

The LE- μ SR measurements at low magnetic field ($B < 1$ mT) allow observing the lower frequency lines of the Mu^0 , since the upper detection limit is about 60 MHz. Interestingly, only one of the Mu^0 states is observed in SiC, as seen for sample Epi-N15 in Fig. 5(a). Since the Mu_1 and Mu_2 have similar hyperfine constants, an overlap of the corresponding frequency lines at 0.7 mT is expected, but only the component corresponding to the Mu_1 is observable: the depolarization rate of the Mu_2 state is with $> 4 \mu\text{s}^{-1}$ [see Fig. 4(c)] too large to be observable in the LE- μ SR spectra with their limited statistics.

Both Mu^0 centers have previously been reported to be isotropic [25], however, the presence of two Mu_1 lines at 0.7 mT for ν_{12} and ν_{23} ($\nu_1 = 9.8$ MHz and $\nu_2 = 11.5$ MHz) indicates a small anisotropy of approximately 1.7 MHz of the Mu_1 hyperfine coupling [18], much smaller than the isotropic part of approximately equal to 3030 MHz [24]. The splitting of the muonium lines is observed for all samples in the low-field and low temperature (10 K) LE- μ SR measurements.

A. Temperature dependence

The temperature dependence investigated in HAL-9500 and in LEM gives insight into the thermally activated processes and charge transitions of muonium in SiC in the temperature range between 10 and 300 K.

The temperature dependence of the muonium formation at 6 T in the bulk of the n-type epilayer with $N_D = 2 \times 10^{14} \text{ cm}^{-3}$ is shown in Figs. 4(b) and 4(c). At 10 K about 100% of the muon polarization is observable, with 29% being in a diamagnetic state, 42% in Mu_1 and 30% in Mu_2 . At approximately 50 K the thermal ionization of the N donors starts [43], leading to the increase of the relaxation rates λ of the diamagnetic and Mu_1 components, and simultaneously the Mu_1 fraction decreases. The Mu_1 center has been assigned to the T_{Si} site next to a Si atom [17,24], where both neutral and negatively charged hydrogen configurations are stable [44,45]. Considering the acceptor character of Mu_1 , electron capture is expected to take place above 50 K, without site change [39]. The variation of the Mu_1 relaxation rate λ_{Mu_1} with temperature was fitted using Eq. (A5) [dashed line in Fig. 4(c)] to extract the capture cross section $\sigma^{0/-}$ of the electron capture process. More details about the fit are included in Appendix A. The decrease in diamagnetic fraction just above 200 K [in Fig. 4(b)] points to the ionization of the Mu^- state with a site change to form Mu_2 [25], whereby the Mu_2 has been assigned to the antibonding site to a carbon atom [25,39].

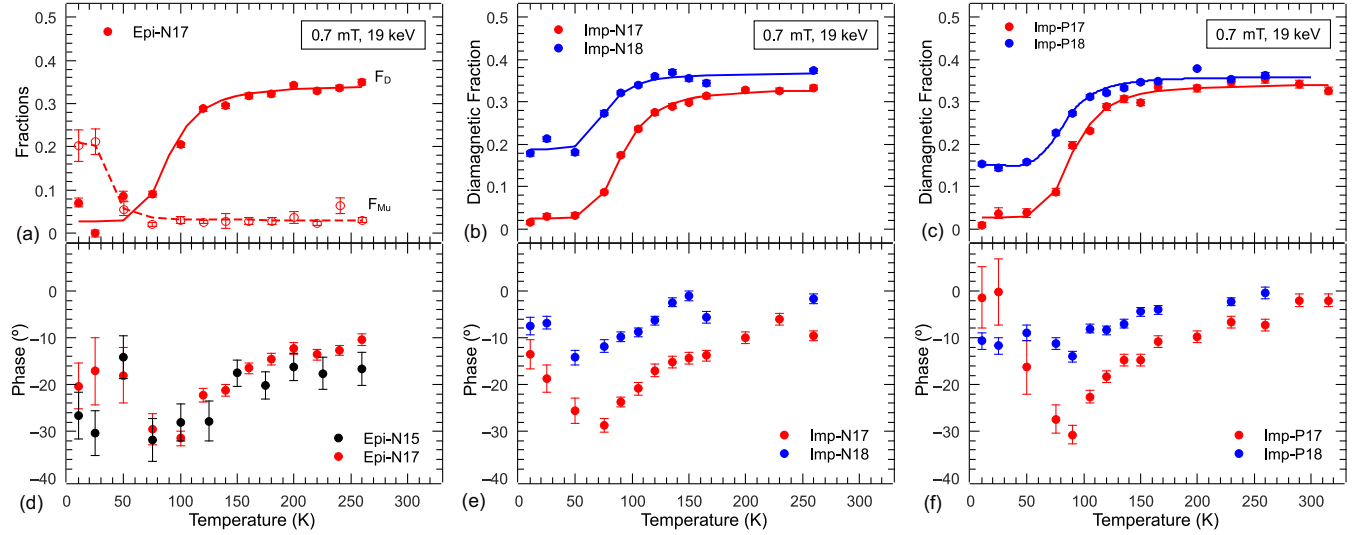


FIG. 6. Muonium fraction F_{Mu} , diamagnetic fraction F_D , and phase ϕ_D measured as a function of temperature for (a,d) Epi-N17. Diamagnetic fraction F_D and phase ϕ_D measured as a function of temperature for (b,e) Imp-N17 and Imp-N18, (c,f) Imp-P17 and Imp-P18. The solid lines show the results of the fits using Eq. (6) to extract the activation energy of the SiC donor species.

The temperature dependence of the different muonium fractions was measured with LE- μ SR at 0.7 mT and 19 keV. For the sample with the lowest doping of $N_D = 4 \times 10^{15} \text{ cm}^{-3}$ (Epi-N15) a small increase of the diamagnetic fraction with temperature was observed in Fig. 5(b), between 10 and 260 K. For this electron concentration, the capture rate λ_c ruling the conversion from Mu^0 to Mu^- is comparable to the lower muonium frequencies, leading to a loss of the initial muon polarization [46] seen in the disappearance of the Mu_1 components [in Figs. 5(b)–5(c)] as its precession becomes unresolved. Thus, the conversion process is not fully observable for this low doping concentration in the SiC. As previously observed, typical F_D values are below 0.1 [17], with the remaining *missing* fraction arising from the fraction of implanted μ^+ that undergo fast depolarization effects.

For the samples with higher doping, the LE- μ SR results of the temperature dependence of the diamagnetic and paramagnetic fractions (F_D and F_{Mu}), and phase ϕ_D are shown in Fig. 6. At low temperatures in the Epi-N17 sample, 20% of muons occupy a Mu_1 state, and 9% form a diamagnetic state, likely Mu^+ . As seen with high-field μ SR, conversion of F_{Mu} to F_D occurs above 50 K, as the donors in SiC start to ionize, and the availability of free carriers contributes to the formation of Mu^- via electron capture. This conversion is seen in Fig. 6(a) as F_{Mu} drops to zero at 50 K, while F_D gradually increases between 50 and 125 K, until the donor ionization is complete and Mu^- formation saturates. The formation of Mu^- usually requires a neutral precursor, which in the case of 4H-SiC is the acceptor Mu_1 , and the process is thus said to be *delayed*. A significant indication of the *delayed* electron capture process is the negative shift in phase

[Figs. 6(d)–6(f)] [21], which is not expected when the diamagnetic state is promptly formed, for example, if the implanted μ^+ remains in the positive Mu^+ state until the decay. The phase shift appears for all samples [in Figs. 6(d)–6(f)] but recovers faster (i.e., is less negative) for the highly doped samples Imp-N18 and Imp-P18. This follows the description of Eq. (5) that electron capture becomes faster with increasing electron availability.

The thermally activated increase of F_D , observed for all samples except Epi-N15, can be fitted with the Boltzmann model from Eq. (6) [47,48], to extract the activation energy E_A of the charge transition process.

$$F_D(T) = f_0 + \frac{b_0 N \cdot e^{-\frac{E_A}{k_B T}}}{1 + N \cdot e^{-\frac{E_A}{k_B T}}}, \quad (6)$$

where f_0 is the diamagnetic fraction at low temperature (< 50 K), N is a density-of-states parameter, b_0 is the interconverting fraction, and k_B is the Boltzmann constant. The values of N used in the fits were fixed to $N = 558$ and $N = 581$ for the epilayer and ion implanted samples, respectively. These N values are the average of the values from fits with free parameters. This model assumes that the temperature provides the activation energy, which is reasonable in the case of the Mu^0 to Mu^- transition because it requires the presence of free electrons, made available by the thermal ionization of the donors in 4H-SiC. Thus, it is expected that the extracted E_A agrees with the energy level of N or P donors in 4H-SiC. The ionization energy depends on whether the donor atoms occupy a cubic (k) or a hexagonal (h) site. For N the energies are 61.4/126 meV and for P 120/60.7 meV in h/k sites, respectively [2,49].

TABLE III. Diamagnetic fractions F_D measured at 10 and 260 K at an implantation energy $E = 19$ keV and a magnetic field $B = 0.7$ mT. The donor activation energy E_A is derived by fitting Eq. (6) to $F_D(T)$ in Figs. 6(a)–6(c).

Sample name	E_A (meV)	F_D (10 K)	F_D (260 K)
Epi-N15	...	0.044(4)	0.091(13)
Epi-N17	61(9)	0.071(10)	0.350(7)
Imp-N17	57(2)	0.016(5)	0.334(6)
Imp-N18	48(5)	0.178(6)	0.374(6)
Imp-P17	57(3)	0.0094(5)	0.353(9)
Imp-P18	53(3)	0.154(5)	0.365(8)

The E_A values obtained from the fits for the different samples are shown in Table III. Only one energy could be extracted, which is assigned to the ionization of the shallower donors, for N in the hexagonal C-site and P in the cubic Si-site.

Under the given measurement conditions, with an applied field of 0.7 mT, we do not observe an increase in the charge carrier concentration due to the ionization of the deeper donors (which are expected to be occupied [2]). This is because neither F_D nor ϕ_D changes significantly within the concentration range of $1 \times 10^{17} \text{ cm}^{-3}$ – $1 \times 10^{18} \text{ cm}^{-3}$. This follows from the simulation discussed below [see Fig. 10(b)]. The E_A for samples with $1 \times 10^{18} \text{ cm}^{-3}$ doping is lower than expected; however, it is in agreement with the electrical characteristics observed in P-implanted SiC, where the ionization energy level decreases with increasing doping concentration [50].

The samples Imp-N18 and Imp-P18 show an increase in F_D compared with Imp-N17 and Imp-P17 at low temperatures, which indicates that more damage is created by the higher fluence implantation (about one order of magnitude larger for Imp-18 than for Imp-17). It is presumed that F_D increases due to either permanent damage created during the implantation, not recoverable by the PIA in Imp-N18 and Imp-P18, or that more atoms are displaced which contribute to an increase of C-related defects during PIA, as seen with LE- μ SR in aluminum implanted samples [20]. The former explanation implies that the higher fluence implantation leads to some amorphization of the lattice, where the likelihood of the incoming muons to stop in a site suitable to form Mu^0 is reduced, hence increasing F_D . The latter involves the displacement of C atoms by the impinging ions, creating V_C , which are not fully annealed out even with the use of the C-cap during annealing, and F_D increases due to the formation of $(V_C\text{-Mu})^-$ complexes [17].

B. Doping profiles after N and P implantation

The depth profiles of the charge carrier concentration were obtained with capacitance-voltage (C-V) measurements, while secondary ion mass spectrometry (SIMS)

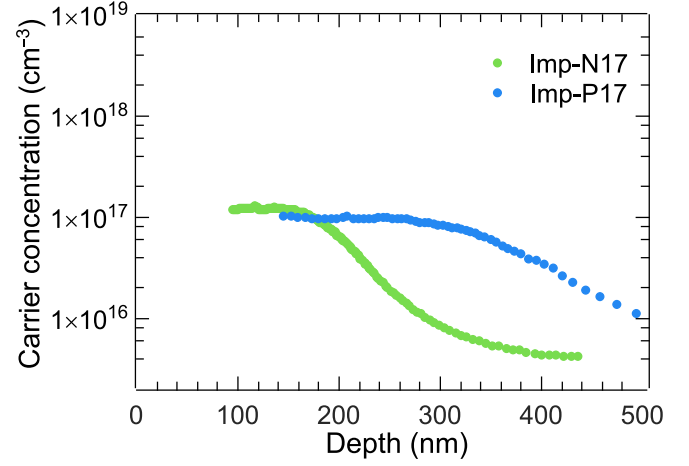


FIG. 7. Depth profiles of the doping concentrations in samples Imp-N17 and Imp-P17, respectively, obtained with capacitance-voltage measurement.

was used to obtain the implanted atom density. The carrier concentration extracted from the C-V is shown in Fig. 7, however, the depth profiles are only measurable for depths higher than 100 nm, and no information on the activation of the dopants near the surface is obtained. For Imp-N17 and Imp-P17, the depth profile of the carrier concentration matches the results of the SRIM simulation (in Fig. 1) and reveals that the dopant activation is close to 100%. Note that the C-V measurements could not be performed on Imp-N18 and Imp-P18 due to a large leakage current; therefore, the electrical activation could not be obtained.

Figure 8 shows the depth profile of the concentrations of N and P atoms in Imp-N18 and Imp-P18, respectively. The depth profiles of the samples Imp-N17 and Imp-P17 could not be accurately determined because the dopant concentration was too close to the lower detection limit of the

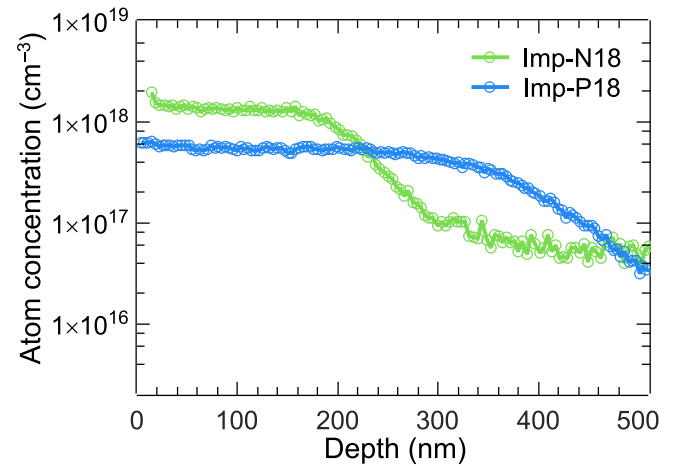


FIG. 8. Depth profiles of N and P concentration in samples Imp-N18 and Imp-P18, respectively, obtained from SIMS.

SIMS tool. Interestingly, the N concentration in the box profile is about twice the concentration of P.

C. LE- μ SR depth analysis

The energy dependence of the muon signal was measured at 260 K, and the fraction and phase of the diamagnetic component are shown in Fig. 9. Although the donors are completely ionized at this temperature, the variation of the F_D with depth suggests the free carrier concentration is not homogeneous over the first 150 nm. For all samples, an increase in F_D at the sample surface is observed. During the slowing down process of the muon, electron-hole pairs are created [52]. However, at low muon implantation energies ($E < 10$ keV) less of these track electrons are generated, which results in an increase in F_D at the sample surface due to the reduced probability to

form Mu^0 from electron capture, and the final state of the muon is Mu^+ [16,22,53]. The increase in F_D at the surface depends on the sample, being 20% in the epilayer samples [Fig. 9(a)] and 40% to 50% in the implanted samples [Figs. 9(b) and 9(c)]. This is attributed to the damage created near the sample surface during the implantation process [18], and additional degradation at the SiC surface due to the annealing process with the C-cap [54]. Furthermore, a thin native oxide layer can form in 4H-SiC due to air exposure of the sample surface [55–57]. The presence of a native oxide on all samples could explain the reduction of F_D setting in at a depth of approximately 10 nm. In this region, the F_D signal is not increasing with temperature, suggesting depletion of electrons. This is unexpected because no metal was deposited on the investigated structures, which would

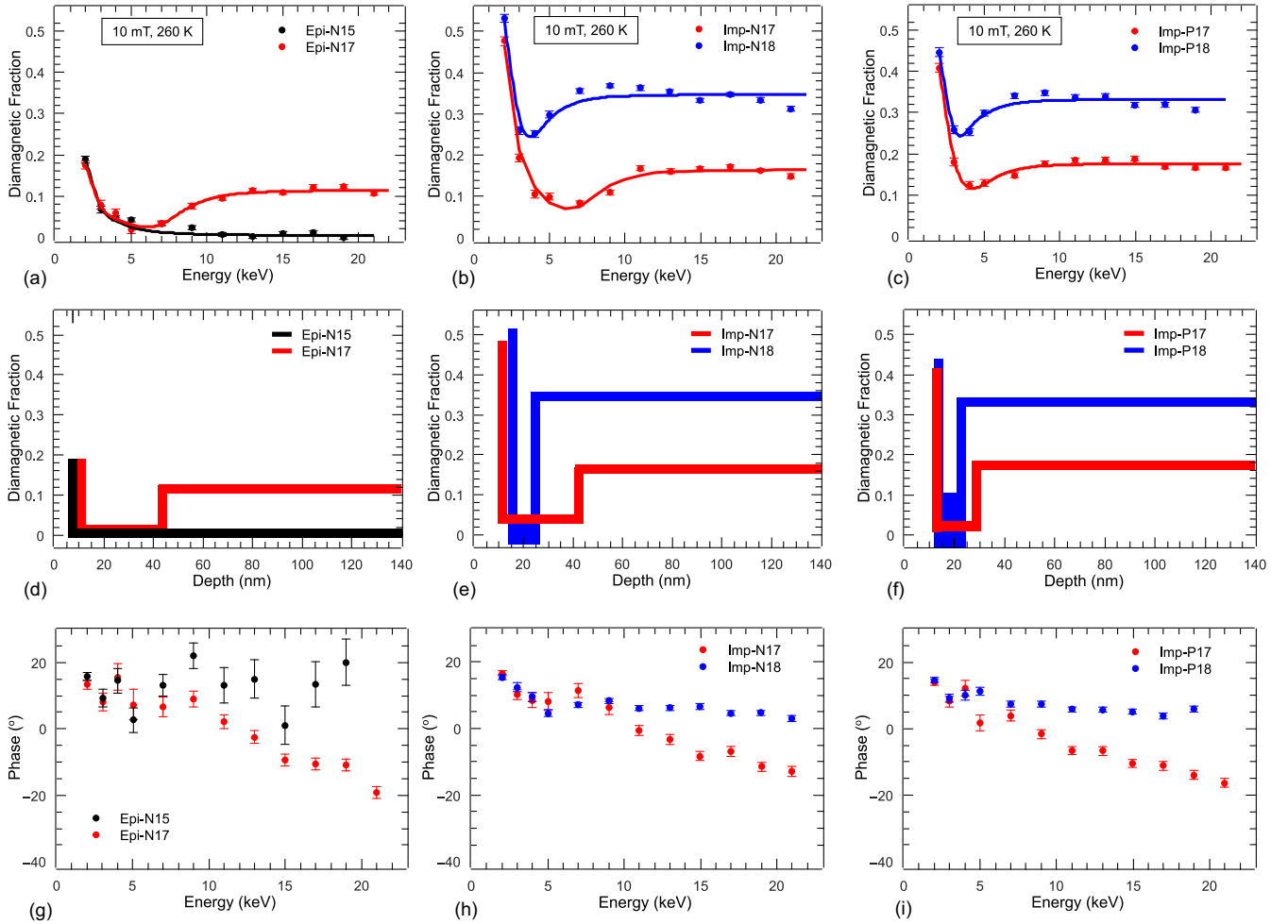


FIG. 9. Diamagnetic fraction F_D as a function of energy and fitted [37,51] assuming the respective depth variation below for (a) epilayer, (b) N-implanted, and (c) P-implanted samples. (d)–(f) The thickness of the lines of the depth variation models represents the standard deviation of the fit parameters. (g)–(i) phase ϕ_D of the diamagnetic signal measured as a function of muon implantation depth. Note that in an applied field of 10 mT, in the absence of muon charge state conversions, ϕ_D is about 15° , compared with about 0° in 0.7 mT in Fig. 6. This difference arises from the different spin precession angles of the low-energy muons in the fringe field of the experimental magnet as they approach the sample.

TABLE IV. Depletion width w_D and diamagnetic fraction F_D recorded at $T = 260$ K and $B = 10$ mT. w_D is the width of the region where a drop in F_D is visible.

Sample name	w_D (nm)	F_D (19 keV)
Epi-N15	...	0.014(4)
Epi-N17	34(3)	0.123(6)
Imp-N17	31(1)	0.163(4)
Imp-N18	8(1)	0.334(5)
Imp-P17	16(1)	0.167(6)
Imp-P18	9(2)	0.319(6)

induce band bending due to the difference in work functions of the different materials. However, band bending in the region between 10 and 40 nm could be induced by charge capture at the SiC surface, possibly in the thin native oxide layer [58]. Interestingly, the width of the region with reduced F_D depends on the doping concentration of the sample, as expected in the case of electron depletion. The depletion width (w_D) values were extracted from the depth models in Figs. 9(d)–9(f), and are summarized in Table IV. The electron depletion was not observed for Epi-N15, since LE- μ SR is not sensitive to an electron concentration as low as $4 \times 10^{15} \text{ cm}^{-3}$ in 4H-SiC. The w_D is expected to depend on the doping concentration, which is seen in the similar values for Epi-N17 and Imp-N17, and the samples with higher doping Imp-N18 and Imp-P18. However, the extracted w_D for Imp-P17 is considerably smaller than for the N17 samples, and is likely due to the difference in the behavior of N and P in the SiC lattice. The presence of V_C with a density greater than $1 \times 10^{17} \text{ cm}^{-3}$ increases F_D [17]. Generation of V_C during ion implantation of Al has been investigated with LE- μ SR, revealing that F_D increases with V_C concentration [20]. Carbon displacement can occur also due to N- and P-implantation, however incorporation of the N-atoms should result in the occupation of the C-site, N_C [59,60], while P-donors are incorporated as P_{Si} . Thus, the increase of F_D due to the presence of unpassivated V_C in Imp-P17 with the formation of $V_C\text{-Mu}^-$ complex does not allow for an accurate extraction of w_D for this sample, since it requires decoupling of the contributions of the C-vacancies and the free electrons to F_D . Furthermore, small deviations between the experimental profiles and the depletion-layer model are observed at larger implantation energies, particularly for the highest-fluence samples Imp-N18 and Imp-P18. Since these deviations become more pronounced with increasing implantation fluence and are accompanied by an enhanced F_D below the depletion region, they are attributed to implantation-induced lattice damage, likely involving the formation of V_C . Beyond the depletion region, the muon signal depends on the doping concentration, as the increase of F_D is accompanied by a phase shift [Figs. 9(g)–9(i)] indicating delayed Mu^- formation in the presence of freeelectrons.

D. Electron capture of Mu in n-type 4H-SiC

With increasing doping concentration, and thus effective free electron concentration, the electron capture process $\text{Mu}^0 + e^- \rightarrow \text{Mu}^-$ leads to an increase of F_D and a negative shift of ϕ_D at 260 K. To model the electron capture process, we employed the simple Monte Carlo simulation described in Sec. II E to calculate μ SR time spectra with statistics similar to the experiment and determined F_D and ϕ_D by fitting the simulated data. In the simulation, only the state transitions involving the Mu_1 state are considered, since it behaves as an acceptor, and as seen in Fig. 4, the electron capture by Mu_1 is the main contributor to the increase of the diamagnetic fraction in n-type SiC.

The diamagnetic fraction F_D and phase ϕ_D measured with LE- μ SR for different doping concentrations (from Table I) were used to calibrate the simulated curves shown in Fig. 10. The diamagnetic fraction [Fig. 10(a)] and phase [Fig. 10(b)] are extracted as a function of capture rate λ_c , and the electron concentration is then calculated

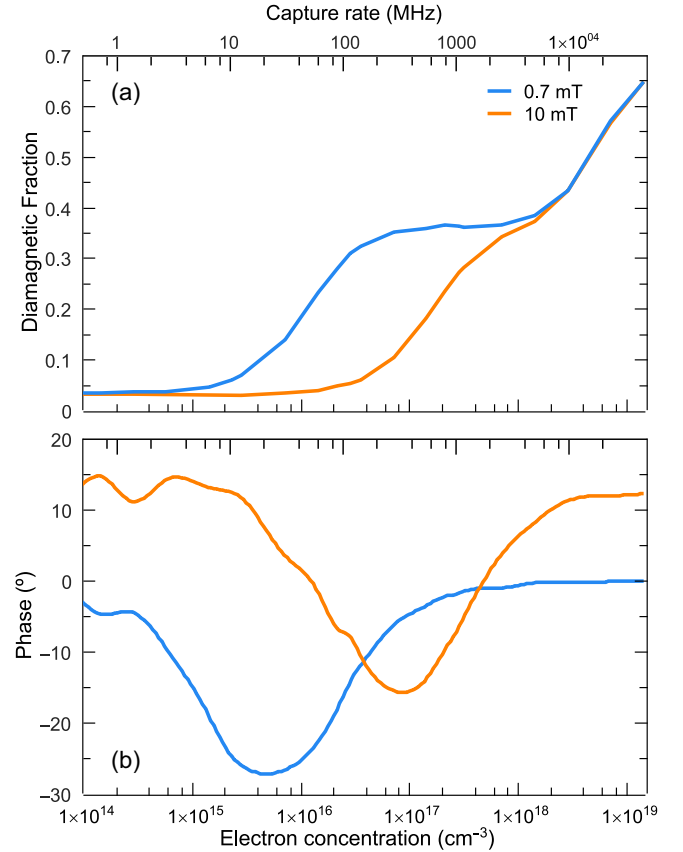


FIG. 10. Simulated dependence of the (a) diamagnetic fraction F_D and (b) phase ϕ_D on the free electron concentration n (at 260 K) and capture rate λ_c for the Mu_1 state with a hyperfine coupling constant $A_{\text{HF}} = 3030$ MHz. At 10 mT, we added in the simulation an offset of $\phi_D = 15^\circ$, to account for the observed spin precession of the muons in the fringe field of the experimental magnet on approaching the sample.

from Eq. (5). To match the collected F_D and ϕ_D to the known free electron concentration, the relation $\sigma^{0/-} \cdot v_e = 3.5 \times 10^{-9} \text{ cm}^3 \text{ s}^{-1}$ was found at a temperature of 260 K.

At 260 K, the thermal velocity v_e of electrons for an effective electron mass of $0.42 \cdot m_e$ is approximately $1.7 \times 10^7 \text{ cm/s}$ (Appendix A). This allows us to estimate the electron capture cross section at 260 K to be $\sigma^{0/-} \sim 2 \times 10^{-16} \text{ cm}^2$, in excellent agreement with the procedure described in Appendix A.

Interestingly, the 10 mT simulated curves of F_D and ϕ_D are shifted to the right compared with the 0.7 mT data, and the increase of F_D starts only at $n \gtrsim 4 \times 10^{16} \text{ cm}^{-3}$, while the presence of $n \gtrsim 2 \times 10^{15} \text{ cm}^{-3}$ already induces a measurable Mu^- fraction at 0.7 mT. This is because a capture rate slower than the Mu^0 frequencies results in the loss of part of the initial muon spin polarization [46]. The low frequency precession lines at 0.7 mT allow to detect the slower electron capture with λ_c on the order of 10 MHz, while $\lambda_c \sim 200 \text{ MHz}$ is in the range of the ν_{12} and ν_{23} frequencies at 10 mT. When electron capture becomes even faster, for $n > 1 \times 10^{18} \text{ cm}^{-3}$, we observe in both magnetic fields a simultaneous increase of F_D , where λ_c becomes larger than the high transition frequencies ν_{34} and ν_{14} of approximately 3000 MHz. Thus, when λ_c is on the order of or faster than any transition frequency of Mu^0 (see Table II) the spin coherence of the muon ensemble is conserved, seen as an increase of F_D and a negative shift of ϕ_D . Once the electron capture becomes sufficiently fast, the polarization loss and dephasing of the diamagnetic component are reduced, and the shift of ϕ_D returns to zero.

The simulated curves of the diamagnetic fraction F_D and phase ϕ_D can be used as calibration curves to quantify the presence of free charge carriers. After establishing the relationship between electron capture rate and carrier concentration using reference samples with known charge carrier density, measurements on an unknown sample can be compared with simulated F_D and phase values obtained under the same magnetic field conditions. Using the results for both 0.7 and 10 mT allows a reliable extraction of the effective electron concentration in the range of 2×10^{15} to $1 \times 10^{19} \text{ cm}^{-3}$, therefore providing a tool for carrier-concentration characterization in 4H-SiC.

IV. CONCLUSION

In this work, the dynamics of muonium in n-type 4H-SiC and the sensitivity of LE- μ SR to different doping concentrations in the range of 4×10^{15} to $1 \times 10^{18} \text{ cm}^{-3}$ were investigated. The temperature-dependent measurements allow the observation of the charge state transition Mu^0 to Mu^- , due to electron capture. Of note, the activation energy of this process was extracted and could be matched to the ionization levels of the donors, revealing the sensitivity of the LE- μ SR parameters to the appearance of free electron carriers. The depth-resolved analysis further uncovered electron depletion regions, likely

induced by fixed charges in a native oxide layer formed at the surface of all the samples.

The samples implanted with N- and P-ions show a comparable electrical activation of the donors, seemingly 100%. However, for a doping concentration of $2 \times 10^{17} \text{ cm}^{-3}$, the P-implantation leads to a higher concentration of V_C compared with N-implantation. The higher fluence used for the doping concentration $1 \times 10^{18} \text{ cm}^{-3}$ also results in permanent damage in the lattice, not recoverable by PIA for both N- and P-implantation, with the main defect candidates being V_C created during ion implantation and C-interstitials related centers during PIA.

The wide range of doping concentrations investigated in n-type 4H-SiC samples, combined with the complete electrical activation of donors following ion implantation, enabled the development of a model linking LE- μ SR observables to free electron concentration. Using a Monte Carlo simulation to describe the electron capture process of Mu^0 in SiC, the variation of the diamagnetic fraction and phase was modeled as a function of electron capture rate. Since the electron capture rate depends on the free electron density, these results establish a method to extract doping levels and carrier concentrations in 4H-SiC through LE- μ SR measurements of the diamagnetic fraction and phase.

ACKNOWLEDGMENTS

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available. The data are available from the authors upon reasonable request.

APPENDIX A: ELECTRON CAPTURE FIT OF Mu_1 RELAXATION RATE

The relaxation rate λ of the Mu_1 state, measured as a function of temperature T in HAL-9500 [Fig. 4(c)], was fitted with Eq. (5). The goal is to extract the activation energy E_A of the process leading to an increase of λ as a function of temperature, and the temperature dependent capture cross section $\sigma^{0/-}$ of the electron capture process for the reaction $\text{Mu}^0 + e^- \rightarrow \text{Mu}^-$. The data were fitted over the temperature range up to 300 K. Above 200 K, the conversion process seems to saturate, and $\lambda(T)$ is approximately constant.

The temperature dependence of the carrier concentration $n(T)$ depends on the ionization of the nitrogen donors with concentration $N_D = 2 \times 10^{14} \text{ cm}^{-3}$ as a function of temperature and is determined by the following function [2]:

$$n(T) = N_D^+(T) = \frac{\gamma(T)}{2} \left(\sqrt{1 + \frac{4N_D}{\gamma(T)}} - 1 \right), \quad (\text{A1})$$

where

$$\gamma(T) = \frac{N_C(T)}{g_D} \exp \left(-\frac{E_C - E_D}{k_B T} \right), \quad (\text{A2})$$

with E_D the donor energy level beneath the conduction band level E_C , g_D the degeneracy factor for donors (taken as 2), and N_C the effective density of states in the conduction band given by

$$N_C = 2M_c \left(\frac{2\pi m_e^* k_B T}{h^2} \right)^{3/2}. \quad (\text{A3})$$

Here, $M_c = 3$ is the number of conduction band minima in the first Brillouin zone [2] and h is Planck's constant. $n(T)$ saturates at $T > 150 \text{ K}$ for an activation energy $E_A = E_C - E_D$ of 60 meV.

For the electron velocity v_e , we assume the electron thermal velocity:

$$v_e(T) = \sqrt{\frac{3k_B T}{m_e^*}}, \quad (\text{A4})$$

where k_B is the Boltzmann constant and $m_e^* = 0.42 \cdot m_e$ [2] is the density-of-states effective mass for electrons.

Since $n(T)$ saturates at $T > 150 \text{ K}$ while $v_e(T)$ is increasing with $\sqrt{T}$, the electron capture cross section $\sigma^{0/-}$ obviously has to decrease with $1/\sqrt{T}$ in this model to yield a constant $\lambda(T)$ at $T > 150 \text{ K}$. The Mu_1 data in Fig. 4(c) were fitted using the function

$$\lambda(T) = \lambda_c(T) = n(T) \cdot v_e(T) \cdot \sigma^{0/-}(100 \text{ K}) \cdot 1/\sqrt{T}. \quad (\text{A5})$$

The free parameters in Eq. (A5) were E_A and $\sigma^{0/-}(100 \text{ K})$, with $E_A = 66(5) \text{ meV}$ and $\sigma^{0/-}(100 \text{ K}) = 3.4(3) \times 10^{-16} \text{ cm}^2$.

E_A fits well to the known activation energy of 61.4 meV of N at the h -site [2].

With the assumed square-root temperature dependence of $\sigma^{0/-}$, we can estimate the expected capture cross section at 260 K to be $\sigma^{0/-}(260 \text{ K}) = \sqrt{100/260} \cdot \sigma^{0/-}(100 \text{ K}) \simeq 2.1 \times 10^{-16} \text{ cm}^2$.

APPENDIX B: TEMPERATURE DEPENDENCE OF THE HYPERFINE COUPLING OF MU IN 4H-SiC

Although this is less relevant to the main message of this article, we would like to include the temperature dependence of the hyperfine coupling of the two muonium states observed in the HAL-9500 data to compare with previous measurements [24]. Data in [24] were for bulk 4H-SiC samples with unknown doping level, indicated as high-resistive, n-type, and p-type, whereas here we have a well-defined epitaxial 4H-SiC layer with n-type doping of $2 \times 10^{14} \text{ cm}^{-3}$.

The hyperfine coupling A_{HF} in Mu^0 is given by [21,30,32]

$$A_{\text{HF}} = \nu_{12} + \nu_{34}, \quad (\text{B1})$$

where $\nu_{12,34}$ are the precession frequencies observed in Fig. 4. As the temperature increases, the long-wavelength acoustic phonons cause a change of the overlap of the Mu^0 $1s$ wave function with the nearest host atoms, resulting in a

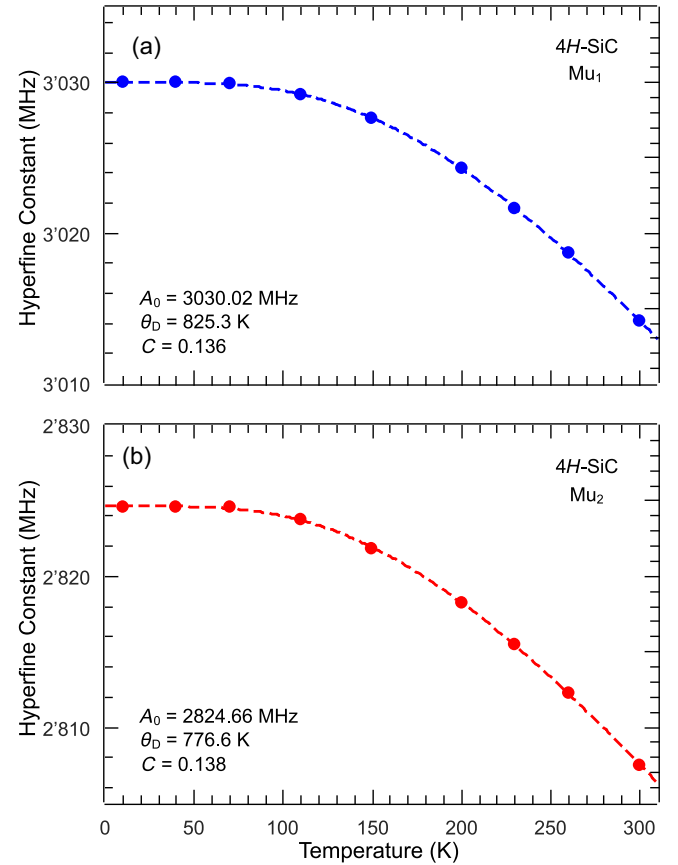


FIG. 11. Hyperfine coupling $A_{\text{HF}}(T)$ as a function of temperature of the (a) Mu_1 and (b) Mu_2 states in n-type ($N_D = 2 \times 10^{14} \text{ cm}^{-3}$) epitaxial 4H-SiC. The dashed lines are fits of Eq. (B2) to the data.

TABLE V. Fitted parameter values for each Mu^0 signal in n-type 4H-SiC, using the Debye model description from Eq. (B2).

Signal	$A_{\text{HF}}(T=0)$ (MHz)	Θ_{D} (K)	C
Mu_1	3030.02(1)	825(9)	0.136(4)
Mu_2	2824.66(3)	776(18)	0.138(7)

reduction of A_{HF} which can be calculated within the Debye model by [24]

$$A_{\text{HF}}(T) = A_{\text{HF}}(0) \cdot \left[1 - C \left(\frac{T}{\Theta_{\text{D}}} \right)^4 \cdot \int_0^{T/\Theta_{\text{D}}} \frac{x^3}{e^x - 1} dx \right], \quad (\text{B2})$$

where C is a dimensionless constant, and Θ_{D} is the Debye temperature. The results for the two Mu states in 4H-SiC are shown in Fig. 11. Additionally, in [24], the fitting of the data for n-type was not possible due to broadening of the Mu^0 signals above 100 K—whereas fitting the HAL-9500 data collected between 10 and 300 K allows extracting reliable parameters.

The parameters resulting from fits to the Mu^0 signals using Eq. (B2) for n-type 4H-SiC are shown in Table V. These parameters are in good agreement with [24]. A lower effective Θ_{D} than the literature value (from specific heat measurements) of 1300 K [24,61] is found, in agreement with [24] and studies on other semiconductors (Si, Ge) [21].

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