Silicon vacancy-type defects in as-received and 12-MeV proton-irradiated 6*H*-SiC studied by positron annihilation spectroscopy

L. Henry, M.-F. Barthe, C. Corbel, P. Desgardin, and G. Blondiaux
Centre d'Etudes et de Recherches par Irradiation, Centre National de la Recherche Scientifique, 3 A rue de la Férollerie, Orléans, France

S. Arpiainen
Laboratory of Physics, Helsinki University of Technology, 02015 HUT, Finland

L. Liszkay
KFKI Research Institute for Nuclear and Particle Physics, H-1525 Budapest 114, P.O. Box 49, Hungary
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Positron lifetime spectroscopy is used to detect vacancy-related defects in as-received and 12-MeV proton-irradiated 6*H*-SiC crystals. We can infer from the temperature dependence of the lifetime spectra decomposition that neutral and negatively charged vacancy defects exist in crystals before and after proton irradiation at low fluence ($\leqslant 4\times10^{15}$ H^+ cm^{-2}). Neutral vacancies are detected after irradiation at high fluence ($\geqslant 4\times10^{16}$ H^+ cm^{-2}). Negatively charged V_{Si} silicon monovacancies with 202 ± 8 ps lifetime are detected at low temperature in as-received *n*-type 6*H*-SiC and after irradiation at low fluence. Neutral $V_{Si\text{-}C}$ divacancies associated with the (225 ± 5)-ps lifetime are produced by irradiation and dominate the positron trapping at room temperature. In addition, different types of ionic acceptors are detected. One of them acts as a strong trapping center even at room temperature.

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I. INTRODUCTION

Silicon carbide is a promising semiconductor material. With its wide band gap and fast switching times, SiC is suitable for high-power and high-frequency electronics and high-temperature applications. SiC occurs in different polytypes.[1] The hexagonal 4*H* and 6*H* polytypes are the most important for microelectronic applications. In this study we concentrate on the 6*H*-SiC polytype, which is the easiest one to produce in good quality. Yet it remains a difficult material to fabricate. Earlier studies clearly show that growth at temperatures far above 1000 °C induces defects that inevitably survive to lower temperatures.[2] This results in a significant defect concentration in the as-grown material, and even more defects are introduced in processing techniques such as ion implantation. Defects in the different polytypes of SiC have been studied by different techniques, including deep-level transient spectroscopy,[1,3] electron spin resonance,[1,4] and positron annihilation spectroscopy.[5–15] In 6*H*-SiC, hydrogen implantation is used for passivation,[16] doping,[17] and the Smart Cut process.[18,19] The nature and the electrical role of the defects that are induced in these implantation techniques are still being discussed. Further work is needed to identify the defects both in as-received and irradiated 6*H*-SiC.

Positron lifetime spectroscopy (PLS) is a powerful technique for investigating the atomic structure and charge states of the defects.[20,21] Positrons get trapped by neutral and negatively charged vacancies and annihilate in associated localized states. As positron lifetime is inversely proportional to the overlap of positron and electron densities at the annihilation site, the lifetime τ_V at the vacancy increases with the open volume. The positron lifetime is thus sensitive to the size of the open volume of the defect. In addition to vacancies, a positron can be trapped at shallow hydrogenic states associated with negative ions. Their lifetime is the same as the lifetime in a lattice. The temperature range of trapping at negative ions depends on their positron binding energy and on their concentration. This trapping at shallow hydrogenic states associated with negative ions leads to a decrease of the fraction of positrons trapped at vacancies.

In this work we use positron lifetime spectroscopy to characterize the vacancy defects in 6*H*-SiC as a function of doping both in the as-received state and after proton irradiation. The measurement of positron lifetime as a function of crystal temperature allowed us to identify different defects and to determine their charge state.

II. EXPERIMENTAL DETAILS

A. 6*H*-SiC crystals and 12-MeV H^+ irradiation

The 22 crystals of $5\times5\times0.3$ mm^3 measured in this study were cut from commercial Cree Research (0001) oriented 6*H*-SiC single crystal wafers. Both nitrogen-doped *n*-type (6*H*-SiC:N, $n=1.9\times10^{17}$ cm^{-3}) and aluminum-doped *p*-type (6*H*-SiC:Al, $p=1.6\times10^{18}$ cm^{-3}) crystals were investigated either in the as-received state or after 12-MeV proton irradiation (Table I). Irradiations were performed using a variable energy cyclotron (CERI-Orléans, France) with fluences varying by two orders of magnitude from 4×10^{14} to 4×10^{15}, 4×10^{16}, and 7.8×10^{16} H^+ cm^{-2}. The particle beam was roughly parallel to the *c* axis of the 6*H*-SiC lattice, and the flux was fixed to 2.6×10^{13} H^+ cm^{-2} s^{-1}. The temperature was maintained at 300 K during irradiation by

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TABLE I. Dopant nature, initial doping level, and 12-MeV proton-irradiation fluences of the SiC crystals studied in this work. The mean positron lifetime and the value $\tau^* = [(I_1/\tau_1) + (I_2/\tau_2)]^{-1}$ are calculated from the decomposition of the spectra measured at 300 K.

Crystal and dopant	Carrier concentration n, p (cm^{-3})	12-MeV H^+ irradiation fluence (cm^{-2})	Mean positron lifetime at 300 K (ps)	τ^* (ps)
6*H*-SiC:Al	$p = 1.6\times10^{18}$	0	145±1	
6*H*-SiC:Al	$p = 1.6\times10^{18}$	4×10^{15}	145±1	
6*H*-SiC:N	$n = 1.9\times10^{17}$	0	150±1	164
6*H*-SiC:N	$n = 1.9\times10^{17}$	4×10^{14}	168±1	184
6*H*-SiC:N	$n = 1.9\times10^{17}$	4×10^{15}	198±1	188
6*H*-SiC:N	$n = 1.9\times10^{17}$	4×10^{16}	207±1	198
6*H*-SiC:N	$n = 1.9\times10^{17}$	7.8×10^{16}	209±1	200

water cooling. The range of 12-MeV protons in 6*H*-SiC calculated with the SRIM program[22] has a value $R_p = 665\ \mu$m. This value is twice the crystal thickness. The 12-MeV protons passed thus through the crystal. The number of C and Si vacancies produced per incident ion and per depth unit is calculated with SRIM as a function of depth. The SRIM calculations have been performed, using as displacement energies in the two sublattices the mean values of the threshold displacement energies calculated by molecular dynamics in SiC by Perlado *et al.*:[23] $E_d(\mathrm{Si}) = 75$ eV and $E_d(\mathrm{C}) = 40$ eV. Note that SRIM does not take into account the recombination processes that could occur during irradiation. This question will be discussed in Sec. V. Assuming that the total vacancy concentration $[V_{\mathrm{tot}}]$ is proportional to the H^+ fluence, we can use the SRIM results to calculate $[V_{\mathrm{tot}}]$ produced as a function of depth at different fluences. In the range 0–300 μm corresponding to the thickness of the H^+-irradiated 6*H*-SiC crystals, the concentration $[V_{\mathrm{tot}}]$ is nearly constant as a function of depth (Fig. 1). It increases from the value 6.5×10^{16} cm^{-3} calculated for the lowest fluence 4×10^{14} H^+ cm^{-2} to the value 1.3×10^{19} cm^{-3} for the highest proton fluence 7.8×10^{16} H^+ cm^{-2} (Fig. 1).

B. Positron lifetime experiments

Positron lifetime measurements were performed using two different conventional fast-fast coincidence spectrometers.[21] The first system has a Gaussian resolution function with a time resolution of 220 ps [full width at half maximum (FWHM)] and has been used to perform lifetime measurements at 300 K. For the second spectrometer a time resolution of 250 ps (FWHM) can be fitted with two Gaussians. This spectrometer has been used for measurements as a function of temperature from 15 up to 300 K. The lifetime spectra were acquired in darkness as a function of the temperature using a closed-cycle He cryocooler. The crystal temperature was first increased in 30-K steps from 15 to 285 K. Then it was decreased from 270 to 30 K by 30-K steps.

A 30-μCi ^{22}Na positron source was sandwiched between two similar crystals. Approximately 2×10^6 events were collected for each spectrum. The lifetime spectra

$$-\frac{dn(t)}{dt} = \sum \frac{I_i}{\tau_i}\exp(-t/\tau_i) \qquad (1)$$

were analyzed as sums of exponential lifetime components τ_i weighted by the intensities I_i, convoluted with the resolution function. The average lifetime is the center of mass of the lifetime spectrum and can be calculated as $\tau_{\mathrm{av}} = \Sigma_i I_i \tau_i$.

III. POSITRON LIFETIME RESULTS

A. As-received 6*H*-SiC

In this section we present the positron lifetime results we obtained as a function of doping in the as-received state.

1. p-type aluminum-doped 6*H*-SiC

The average lifetime in the four as-grown *p*-type 6*H*-SiC:Al crystals is about 145 ps at room temperature (see Table I). It remains constant as a function of temperature. Two lifetime components can be detected. At room temperature, the τ_1 short component lifetime has the value 140 ±5 ps and the τ_2 long component lifetime is 190±10 ps and intensity I_2 has the value 20±10 %. These components are independent of temperature in the 15–300-K range.

2. n-type nitrogen-doped 6*H*-SiC

In the four as-received *n*-type 6*H*-SiC:N crystals, the average positron lifetime τ_{av} changes as a function of measurement temperature [Fig. 2(a)]. The average positron lifetime has the value $\tau_{\mathrm{av}} = 150\pm1$ ps at room temperature (see Table I). When the temperature decreases, it goes through a maximum of 156 ps measured at about 45 K. τ_{av} decreases down

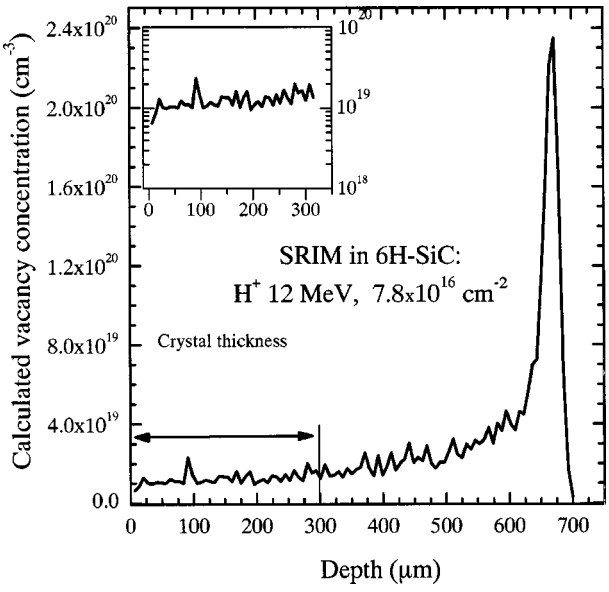

FIG. 1. Total concentration of vacancies induced by 12-MeV proton irradiation at 7.8×10^{16} H^+ cm^{-2} as a function of depth in 6*H*-SiC as calculated by SRIM (Ref. 22).

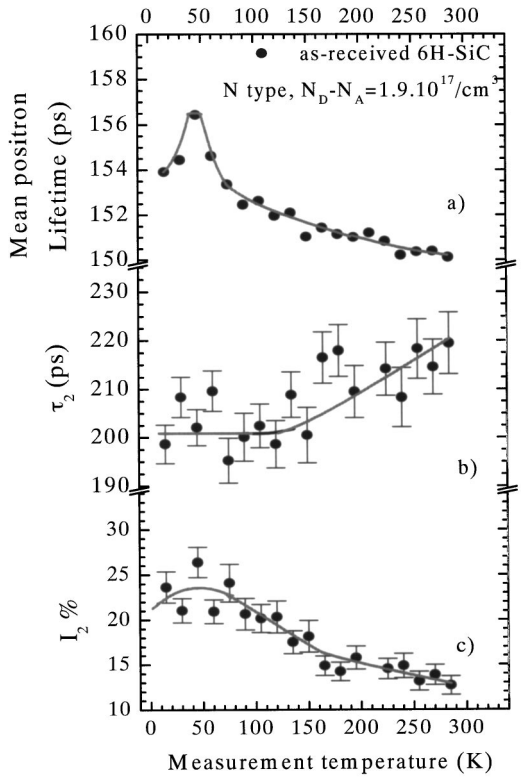

FIG. 2. Temperature dependence of the positron lifetime parameters in as-received *n*-type 6*H*-SiC:N: (a) mean lifetime τ_{av}; (b) lifetime τ_2 of the longer component; (c) its intensity. The lifetime τ_1 of the shortest component is 140 ± 5 ps at all temperatures. The solid lines are guides to the eye.

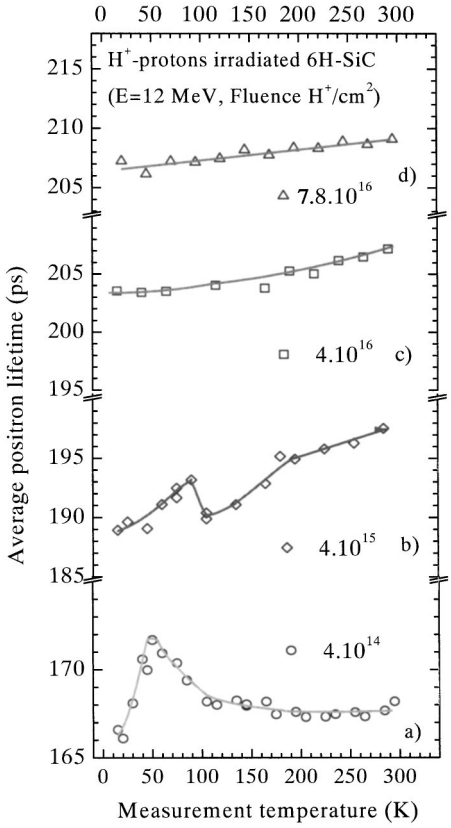

FIG. 3. Temperature dependence of the positron mean lifetime τ_{av} in 12-MeV proton-irradiated *n*-type 6*H*-SiC:N for different incident particle fluences: (a) 4×10^{14} H$^+$ cm^{-2}, (b) 4×10^{15} H$^+$ cm^{-2}, (c) 4×10^{16} H$^+$ cm^{-2}, and (d) 7.8×10^{16} H$^+$ cm^{-2}. The solid lines are guides to the eye.

to 154 ps for the lowest temperature (15 K). All the lifetime spectra can be decomposed into two components. The short lifetime component τ_1 is of 140 ± 5 ps at room temperature and remains constant when temperature decreases. The long component lifetime is $\tau_2=216\pm6$ ps at 300 K. τ_2 decreases with temperature down to a plateau value of 202 ± 8 ps measured in the 15–150 K temperature range [Fig. 2(b)]. The long component intensity I_2 behaves as the average lifetime. I_2 is of 12 ± 2 % at room temperature and goes through a maximum of 27 ± 2 % at 45 K [Fig. 2(c)]. I_2 decreases when temperature decreases between 45 and 15 K.

B. 12-MeV proton-irradiated 6*H*-SiC

In the following we examine the lifetime results as a function of doping in 6*H*-SiC after 12-MeV proton irradiation.

1. p-type aluminum-doped 6*H*-SiC

In proton-irradiated *p*-type 6*H*-SiC:Al crystals, the average positron lifetime is independent on the fluence at least up to the irradiation fluence of 4×10^{15} cm^{-2}. The decomposition remains identical to the one measured in the as-received state. The spectra are independent of temperature.

2. n-type nitrogen doped 6*H*-SiC

In 12-MeV proton-irradiated *n*-type 6*H*-SiC:N, the average positron lifetime measured at room temperature increases monotonically with increasing fluence (Table I). The average lifetime increases from $\tau_{av}=150\pm1$ ps to $\tau_{av}=209\pm1$ ps at room temperature for the highest fluence of 7.8×10^{16} H$^+$ cm^{-2}. Whatever the fluence is, the lifetime spectra as a function of temperature are always resolved into two components (τ_i, I_i). The decomposition behavior as a function of temperature changes with the proton fluence.

After irradiation at the lowest fluence of 4×10^{14} H$^+$ cm^{-2}, τ_{av} depends on temperature [Fig. 3(a)]. From the value 166 ± 1 ps at 15 K, τ_{av} goes through a maximum of 172 ± 1 ps measured at 55 K. Then τ_{av} reaches 167.5 ± 1 ps at 200 K and remains constant up to room temperature. The two exponential components resolved in the spectra have different temperature dependences. The short lifetime component is about 140 ± 5 ps at 300 K and remains constant when temperature changes in the 15–300 K range. The long lifetime component τ_2 decreases with decreasing temperature by 12 ps from the value 225 ± 2 ps at room temperature to the value 213 ± 2 ps at 15 K [Fig. 4(a)]. The long component intensity I_2 behaves as the average lifetime. It has a value of 32 ± 3 % at 300 K and when temperature decreases I_2 goes through a small maximum of 43 ± 2 % at 55 K [Fig. 4(b)]. I_2 reaches the value 34 ± 3 % at 15 K.

After irradiation at 4×10^{15} H$^+$ cm^{-2} fluence τ_{av} has the value 190 ± 1 ps at 15 K. With increasing temperature, it

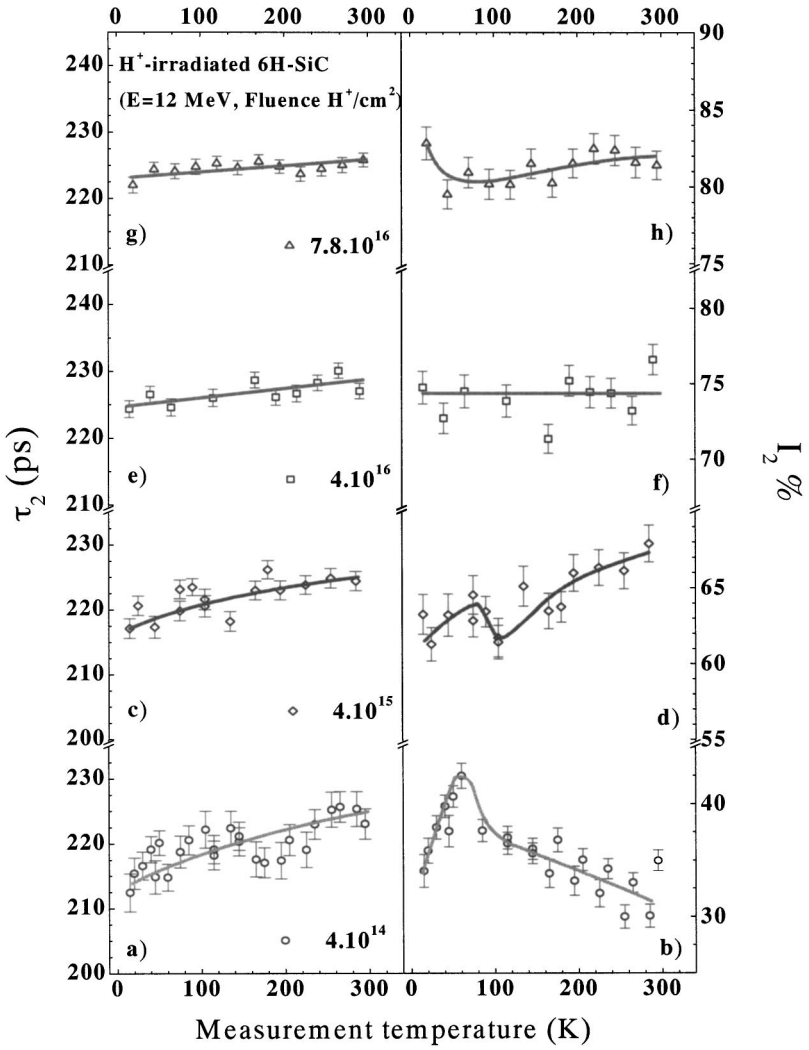

FIG. 4. Temperature dependence of the positron lifetime spectra decomposition in 12-MeV proton-irradiated *n*-type 6*H*-SiC:N. The lifetime τ_2 of the longer component and its intensity I_2 are shown, respectively, on the left and right panel for different incident particle fluences: (a) and (b) 4×10^{14} H^+ cm^{-2}, (c) and (d) 4×10^{15} H^+ cm^{-2}, (e) and (f) 4×10^{16} H^+ cm^{-2}, and (g) and (h) 7.8×10^{16} H^+ cm^{-2}. The lifetime of the shortest component τ_1 is 140 ± 5 ps at all temperatures. The solid lines are guides to the eye.

goes through a maximum of 193 ps around 90 K and reaches 198 ± 1 ps at room temperature [Fig. 3(b)]. The two exponential components resolved in the spectra have different temperature dependence. The short lifetime component is of about 140 ± 5 ps at room temperature and remains constant when temperature changes in the 15–300-K range. The long lifetime component is $\tau_2=226\pm2$ ps at room temperature and decreases to 219 ± 2 ps at 15 K [Fig. (4c)]. The long lifetime component intensity I_2 shows the same features as the average lifetime [Fig. 4(d)]. At room temperature I_2 has the value 67 ± 3 %. When the temperature decreases I_2 decreases to a minimum of 62 ± 2 % at 15 K going through a small maximum of 64 ± 2 % around 90 K [Fig. 4(d)].

After irradiation at 4×10^{16} H^+ cm^{-2}, τ_{av} increases monotonically with increasing temperature. At 15 K the value is $\tau_{av}=204\pm1$ ps (see Table I) and reaches 207 ± 1 ps at room temperature [Fig. 3(c)]. The decomposition is slightly temperature dependent. The short lifetime component is of about 140 ± 5 ps and remains constant when the temperature changes in the 15–300-K range. τ_2 slightly decreases with temperature [Fig. 4(e)] from $\tau_2=229\pm2$ ps at room temperature to $\tau_2=225\pm2$ ps at 15 K. At room temperature the long lifetime component intensity I_2 is $I_2=74\pm2$ % and remains approximately constant when temperature decreases [Fig. 4(f)].

After irradiation at the highest fluence of 7.8×10^{16} H^+ cm^{-2} the average lifetime increases with increasing temperature by 2 ps from 207 ± 1 ps at 15 K to 209 ± 1 ps at 300 K. Both lifetime components resolved in the spectra remain constant as a function of temperature in the 15–300-K range. The short lifetime τ_1 is of about 140 ± 5 ps. The long component τ_2 has a value of $\tau_2=226\pm2$ ps at room temperature and intensity $I_2=82\pm1$ % [Figs. 4(g) and 4(f)]. τ_2 and I_2 remain constant when temperature decreases.

In summary there are two types of temperature dependence for the average lifetime in the irradiated *n*-type 6*H*-SiC crystals depending on the proton fluence. There is a maximum after low fluence irradiation at 4×10^{14} and 4×10^{15} H^+ cm^{-2}. For all fluences there is a slight increase with increasing temperature after high fluence irradiation at 4×10^{16} and 7.8×10^{16} H^+ cm^{-2}. The short lifetime τ_1 is of about 140 ± 5 ps at 15 K and remains constant when temperature increases in the 15–300-K range. Depending on the fluence, the values of τ_2 at low temperature, 15 K, vary from 213 ± 2 ps for the lowest fluence irradiation at 4

$\times 10^{14}$ H^+ cm^{-2} to 226 ± 2 ps for the highest fluence irradiation at 7.8×10^{16} H^+ cm^{-2}. Whatever the proton fluence is, the τ_2 lifetime is 226 ± 3 ps at room temperature. The long component intensity I_2 obtained at 300 K increases with increasing proton fluence from $I_2 = 32 \pm 3$ % at the low fluence of 4×10^{14} H^+ cm^{-2} to 82 ± 2 % at the high fluence of 7.8×10^{16} H^+ cm^{-2}.

IV. DISCUSSION

In this section we discuss the lifetime results as a function of doping type both in the as-received and the irradiated state.

A. *p*-type aluminum-doped 6*H*-SiC: 1.6×10^{18} cm^{-3}

In the temperature range from 15 to 300 K, the average lifetime in as-received highly doped *p*-type 6*H*-SiC is 5 ps longer than the 140-ps lifetime characteristic of annihilation in the 6*H*-SiC lattice as calculated[10,24,25] or measured by different authors.[11,13,26–30] It indicates that vacancy defects are present in the crystal. The decomposition suggests that the lifetime value arising from annihilation in the vacancy defect is 190 ± 10 ps. As described in Ref. 31, the value $\tau^*(T) = [I_1(T)/\tau_1(T) + I_2(T)/\tau_2(T)]^{-1}$ is equal to the lifetime characteristic of annihilation in the lattice when a model with only one vacancy-type defect can be used to describe positron trapping. In the *p*-type material, $\tau^*(T)$ calculated from the spectra decomposition has the value 148 ps and is temperature independent. $\tau^*(T)$ is longer than 140 ps, indicating that positrons are trapped in different types of defects. The decomposition shows that at all temperature Δ the short lifetime is equal to 140 ps. This value corresponds to lattice annihilation. As shown in Ref. 31, such behavior in the presence of trapping at vacancy-type defects can be attributed to positron trapping at negative ions.

The comparison of the lifetime at the vacancy-type defects with values calculated in 6*H*-SiC (Ref. 25) suggests that the lifetime is due to a monovacancy. In this highly Al-doped material, these vacancies are still neutral or negatively charged since they are detected by positrons. This property suggests that they are vacancy-Al complexes. The negative ions in this highly Al-doped material can be the Al acceptors. However, another type of negative ion cannot be excluded since, as seen below, trapping at negative ions is also detected in *n*-type 6*H*-SiC.

In proton-irradiated *p*-type SiC crystals, the average positron lifetime remains at the as-grown value at least up to the irradiation fluence of 4×10^{15} cm^{-2}. Data showing that the lifetime starts to increase at higher fluences will be published and discussed elsewhere.[32] This fluence effect suggests that in *p*-type material the irradiation-induced vacancy defects are probably in a positive charge state, when the Fermi level is close to the valence band. It is well established that such positive vacancy defects repel positrons and remain undetected.[33]

B. *n*-type nitrogen-doped 6*H*-SiC

1. As-received *n*-type nitrogen-doped 6*H*-SiC: 1.9×10^{17} cm^{-3}

In the temperature range from 15 to 300 K, the average lifetime in as-received *n*-type 6*H*-SiC is longer than the 140 ps lifetime characteristic of annihilation in the 6*H*-SiC lattice, indicating that vacancy defects are present in the crystal. The values $\tau^*(T) = [I_1(T)/\tau_1(T) + I_2(T)/\tau_2(T)]^{-1}$ calculated at all temperatures from the spectra decomposition are much longer than 140 ps, indicating that positrons are trapped in different types of defects.[31]

The existence of various types of vacancy defects is clearly displayed in Figs. 2(a) and 2(b) by the variation of the average lifetime $\tau_{av}(T)$ and of the long lifetime $\tau_2(T)$ as a function of temperature. In Fig. 2(b) the decrease of $\tau_2(T)$ with decreasing temperature reflects that temperature induces strong variations in the trapping rates $k_j = \mu_j c_j$ of the vacancy defects constituting the distribution. The change in k_j with temperature can result from a change in the defect concentration c_j with temperature and/or from a change in the trapping coefficient μ_j with temperature. The concentration of defects can vary in a semiconductor as a function of temperature when the Fermi level crosses one of their ionization levels. The as-received SiC:N wafer used for this study is highly doped $n_D - n_A = 1.9 \times 10^{17}$ cm^{-3}. The electron levels are filled up to the nitrogen ionization level at $E_C - 0.2$ eV. As the temperature changes, the Fermi level remains nearly constant in a so highly doped SiC material. Consequently, we can assume that the charge state of defects is constant as a function of temperature in the 15–300-K range. We are left to conclude that the temperature dependence $\tau_2(T)$ reflects the presence of at least two types of vacancy defects.

A vacancy defect with a long lifetime longer or equal to 216 ± 5 ps is detected at room temperature. A smaller one with a shorter lifetime of 202 ± 8 ps is detected at low temperature. The trapping coefficient of vacancy defects is known to increase with the size of the vacancy defect.[18,31] In order to compete with the trapping in the largest defect, the trapping coefficient μ at the smallest defect has to increase when temperature decreases. This property is fulfilled for negatively charged defects where the trapping coefficient μ from the lattice to the deep localized states are known to change in $T^{-1/2}$.[33] We propose that the decrease in the τ_2 lifetime observed at low temperature (from around 150 K) arises from trapping at negatively charged vacancies. The lifetime characteristic of annihilation at negatively charged vacancies is equal to the τ_2 plateau value of 202 ± 8 ps measured in the 15–100-K range. The τ_2 lifetime value, 216 ± 5 ps, measured at room temperature is due to trapping at neutral vacancy defects.

The τ_1 short lifetime measured around 140 ps in the as-received *n*-type crystals has the same value as the lifetime characterizing the annihilation in the 6*H*-SiC lattice. As described in Ref. 31, it suggests that positrons are trapped at negative ions. These negative ions, which are detected up to room temperature, are referred as $A^-_{300\,K}$. The trapping at these negative ions compete with trapping at vacancy defects up to at least room temperature. Such a behavior suggests that as it was demonstrated in Ref. 34, the $A^-_{300\,K}$ concentra-

tion or/and its positron binding energy are high.

Moreover, in addition to $A^-_{300\,K}$ ions, the I_2 decrease observed when the temperature decreases below 45 K suggests the existence of other negative ions that act below 45 K and are referred as $A^-_{15\,K}$. The nature of these shallow traps $A^-_{15\,K}$ is different from the negative ions $A^-_{300\,K}$ that trap positrons even at 300 K. The positron binding energy to $A^-_{15\,K}$ ions or/and the $A^-_{15\,K}$ concentration are much lower than that for $A^-_{300\,K}$.

2. 12-MeV proton-irradiated n-type 6*H*-SiC

After 12-MeV proton irradiation, the increase of the average positron lifetime with increasing fluence shows the creation of vacancy defects (Table I). In all the irradiated crystals, the values $\tau^*(T)=[I_1(T)/\tau_1(T)+I_2(T)/\tau_2(T)]^{-1}$ calculated at all temperatures from the spectra decomposition are much longer than the 140-ps value characteristic of annihilation in the 6*H*-SiC lattice, indicating that positrons are trapped by different types of defects.

In the crystals irradiated at the lowest fluence, the existence of various types of vacancy defects is clearly displayed by the variation of the average lifetime $\tau_{av}(T)$ as a function of temperature in Fig. 3(a) and of the long lifetime $\tau_2(T)$ in Fig. 4(a). As we discussed, for the as-received crystal (see Sec. IV B 1), the decrease of $\tau_2(T)$ as temperature decreases reflects that temperature induces strong variations either in the defect concentration c_j and/or in the trapping coefficient μ_j. EPR measurements performed by von Bardeleben *et al.*[35] have shown that the crystals remain, after 4×10^{14} H^+ cm^{-2} proton irradiation, as *n* type with their electron levels filled up to a Fermi level position close to the nitrogen ionization level at $E_C-0.2$ eV. As in the as-received crystals, we can assume that the charge of defects is constant as a function of temperature in the 15–300-K range. So we can conclude that the $\tau_2(T)$ decrease with decreasing temperature is due to positron trapping at two types of vacancy defects with different sizes and different charge states. A vacancy defect with a long lifetime $\geqslant 225\pm5$ ps is detected at room temperature and a smaller one with a shorter lifetime $\leqslant 213\pm2$ ps induces the τ_2 decrease at low temperature. On the basis of the arguments used in Sec. IV B 1 we propose that the charge states associated with these two types of defects are different. The small defect with lifetime $\tau_V \leqslant 213\pm2$ ps, which appears at low temperature, has a negative charge state. The larger defects with lifetime $\tau_V \approx 225 \pm 5$ ps that dominate trapping at room temperature have a neutral state.

After irradiation at the middle fluence of 4×10^{15} H^+ cm^{-2}, the τ_2 change as a function of temperature indicates also competition between trapping at different vacancy defects of different size and different charge states. Neutral vacancy defects with large lifetimes $\geqslant 225\pm5$ ps trap the positron at room temperature, whereas negatively charged smaller defects of lifetimes $\leqslant 219\pm2$ ps influence the trapping at low temperature more.

After irradiation at the highest fluences of 4×10^{16} and 7.8×10^{16} H^+ cm^{-2}, the lifetime is roughly temperature independent. It suggests that the same vacancy defects giving rise to the lifetime 226 ± 4 ps dominate positron trapping at all temperatures.

We notice that the lifetime 226 ± 4 ps is detected at room temperature in all the proton-irradiated crystals, whatever the fluence. In addition, it is constant as a function of temperature after high fluence irradiation. Such features suggest that this lifetime corresponds to annihilation in a unique type of vacancy defect more than in a distribution of different types of defects. Furthermore, considering our previous discussion, we can reach the conclusion that this defect is neutral.

The τ_2 values at low temperature vary with fluence. The minimum measured value is 213 ± 2 ps for the lowest fluence of 4×10^{14} H^+ cm^{-2}. Consequently, the lifetime of the negatively charged vacancy defects that we associated with trapping at low temperatures is equal to or shorter than the (213 ± 2)-ps value. Once we assume the existence of neutral and negatively charged defects, the effect of proton fluence on the temperature dependence of the lifetime $\tau_2(T)$ can be ascribed to a fluence-dependent competition between trapping at neutral and negative defects. When fluence increases, the trapping at neutral defects progressively overcomes the trapping at negatively charged defects at all temperatures. This possibly reflects that the Fermi level drops below the ionization levels of the small defects after high-fluence irradiation. Some EPR measurements suggest a strong reduction in ionized nitrogen concentration after high-fluence irradiation.[35]

As we proposed in Sec. IV B 1 for the as-received *n*-type crystals, the short lifetime values τ_1 around 140 ps measured in all the proton-irradiated crystals is attributed to positron trapping at negative ions. These negative ions are detected up to room temperature whatever the proton fluence.

The long component intensity I_2 increases below 60 and 75 K after irradiation at the low fluences of 4×10^{14} and 4×10^{15} H^+ cm^{-2}, respectively. The decrease in I_2 is observed from 60 and 75 K, respectively. We attribute it to another type of negative ion than the negative ion $A^-_{300\,K}$.

V. NATIVE AND 12-MeV PROTON-IRRADIATION-INDUCED VACANCIES

In the preceding section, we have seen that the positron lifetime of about 202 ps can be attributed to a negatively charged vacancy defect that is observed at low temperature in *n*-type as-received 6*H*-SiC crystals. The positron lifetime of 225 ps is characteristic of the neutral vacancy-type defects that are induced in *n*-type 6*H*-SiC by 12-MeV proton irradiation. This 225-ps defect dominates the trapping at room temperature in all crystals irradiated with different fluences. After irradiation at the lowest fluences another type of vacancy defect is detected at low temperature. This defect is negatively charged and has a lifetime equal to or shorter than 213 ps.

Theoretical calculations give quantitative estimates of the positron lifetimes in various annihilation states. According to the recent results of Staab *et al.*,[25] the calculated lattice lifetime is 131 ps, which is in reasonable agreement with the present experimental value of 140 ps. Taking into account the relaxations of atoms around vacancies,[36] a lifetime in-

crease of a factor $(\tau_{V_C}-\tau_L)/\tau_L=0.05$ can be expected for the C vacancy and $(\tau_{V_{Si}}-\tau_L)/\tau_L=0.485$ for the Si vacancy.[25] When scaled with our experimental value $\tau_L=140$ ps, the theory thus predicts positron lifetimes of $\tau_{V_C}=147$ ps and $\tau_{V_{Si}}=203$ ps for V_C and V_{Si}, respectively. $\tau_{V_{Si}}=203$ ps is very close to the experimental values that characterize negatively charged vacancy defects observed in *n*-type as-received crystals (202 ± 8 ps), thus supporting the identification of Si vacancies. In this work we propose that the 202-ps lifetime corresponds to the annihilation at V_{Si} which is in agreement with that reported by Kawasuso *et al.*[13] but slightly lower than the value Müller *et al.*[37]

Furthermore, the calculation predicts that the positron lifetime at $V_{C\text{-}Si}$ divacancies is about 223 ps [$(\tau_{V_{C\text{-}Si}}-\tau_L)/\tau_L=0.594$ for the C-Si divacancy],[25] which is very close to the lifetime of the dominating vacancy defect produced by proton irradiation, 226 ± 4 ps. Defects with lifetime 222 ± 9 ps, similar to what we obtain in this work, have been observed by Polity, Huth, and Lausmann[11] after irradiation with 2-MeV electrons at 4 K. The authors suggest that this lifetime is due to positron trapping at $V_{C\text{-}Si}$ divacancies. In 3-MeV electron-irradiated 6*H*-SiC at 1.5×10^{18} e^- cm^{-2} fluence, Kawasuso *et al.*[28] observed a lifetime of 215 ps at room temperature. They associated this lifetime to strong trapping at $V_{C\text{-}Si}$ divacancies formed during irradiation. We propose that the $V_{C\text{-}Si}$ divacancy characterized by the 226 ± 4 ps lifetime is produced by proton irradiation and dominates the positron trapping at room temperature.

In low fluence $\leqslant4\times10^{15}$ H^+ cm^{-2} proton-irradiated crystals, a negatively charged vacancy defect with a lifetime $\tau_V\leqslant213$ ps competes at low temperature with the 225-ps vacancy-type defect. We propose that the trapping at low temperature arises from a negatively charged Si vacancy. It is supported by some positron annihilation experiments performed under monochromatic light excitation. From these experiments, it has been inferred that Si vacancies have ionization levels at $E_C-0.6$ eV and $E_C-1.2$ eV that have been associated with (2−/1−) and (1−/0), respectively, ionizations of the isolated Si vacancy.[38] In the low-fluence irradiated crystals, V_{Si} can thus exist in the 2− charge state since EPR measurements[35] have shown that the Fermi level is located close to the nitrogen ionization level at $E_C-0.2$ eV.

At high fluences $\geqslant4\times10^{16}$ H^+ cm^{-2}, we can consider two processes that can explain the absence of detection of the negatively charged defects: (i) The charge state of the ⩽213 ps defect becomes more positive as fluence increases, and/or (ii) the ratio of production of the 225-ps defect to the production of the ⩽213-ps defect increases with fluence. Concerning the first process, EPR signals[35] have indeed been assigned to silicon vacancies in the neutral and negative charge state only after irradiation at the highest fluences ($\geqslant1\times10^{16}$ H^+ cm^{-2}).

The relative V_{Si} concentrations in different states have been determined. At 7.8×10^{16} H^+ cm^{-2} fluence the V_{Si}^- concentration is about 1.02×10^{18} cm^{-3} and the V_{Si}^0 concentration reaches 1.42×10^{18} cm^{-3}. The appearance of a more positive charge state induces a decrease in positron trapping due to the decrease of the trapping coefficient. According to the calculations performed by Puska, Corbel, and Nieminen[33] for trapping coefficients at different defects in Si the trapping coefficient at 15 K is expected to decrease by a factor of about 2 when the V_{Si} charge state changes from 2− to 1− and 50 for the charge change from 2− to 0.[33] In the following we assume that the ratios of the trapping coefficients for the different types of vacancies in 6*H*-SiC are of the same orders as the theoretical values given by Puska, Corbel, and Nieminen[33] for the corresponding types of vacancy in silicon. Consequently, one can estimate that the mean trapping coefficient at the V_{Si} monovacancy at the temperature 15 K

$$\bar{\mu}_{V_{Si}}=(\mu_{V_{Si}^-}[V_{Si}^-]+\mu_{V_{Si}^0}[V_{Si}^0])/([V_{Si}^-]+[V_{Si}^0])$$

decreases by a factor of about 6 when irradiation fluences increase to 7.8×10^{16} H^+ cm^{-2}. To comment on the second process, one need to estimate the divacancy concentrations produced at high proton fluence. Let us notice that the V_{Si}^- concentration determined by EPR[35] is quite high at the value 1.02×10^{18} cm^{-3} for 7.8×10^{16} H^+ cm^{-2} fluence. In these irradiated crystals divacancies are still able to compete with the V_{Si}^- concentration even at low temperature, where, according to calculations in Si, the ratio of the trapping coefficient $\mu_{V_{Si}^-}/\mu_{V_{C\text{-}Si}^0}$ in 6*H*-SiC is expected to be higher than 15 at 15 K. It follows that on this basis the concentration of the $V_{C\text{-}Si}$ divacancies produced at 7.8×10^{16} H^+ cm^{-2} fluence can reach 1×10^{19} cm^{-3}. This value is in the same range as that of the total concentration of vacancies calculated by SRIM. It suggests that the $V_{C\text{-}Si}$ divacancy is the dominant vacancy defect that is created by 12-MeV proton irradiation. Similar conclusions have been drawn in a study performed on 5-MeV proton-irradiated *n*-type 6*H*-SiC.[39]

In SiC the vacancy-interstitial recombination rate during irradiation is still poorly known. It depends on the irradiation conditions (temperature, flux, etc.). From the present results we can evaluate the total concentration of vacancies that exist under the forms of V_{Si} vacancy or $V_{C\text{-}Si}$ divacancies. It is given by the relation $[V]_{tot}\approx[V_{Si}]+2[V_{C\text{-}Si}]\approx2\times10^{19}$ cm^{-3}. This value is about twice the value given by SRIM calculations and consequently appears to be overestimated. It should be noticed that the present estimation relies on the EPR value of the V_{Si} vacancy concentration[35] and on the estimated value of the ratio of the monovacancy V_{Si} and divacancy $V_{C\text{-}Si}$ positron trapping coefficients in 6*H*-SiC. Assuming that the EPR estimation for the V_{Si} concentration is correct, we are led to revise the value that can be attributed to the ratio of the trapping coefficients. A value of 7, still consistent with theory, gives a fair agreement between the SRIM calculations of the vacancy concentration and the present experimental determination. Another conclusion that can be drawn from the present results is that the recombination of vacancy with interstitial seems to be rather low.

As it has been discussed in Ref. 35 the V_{Si} concentrations determined by EPR are much lower than the values calculated with SRIM. The authors attributed this difference to the interstitial monovacancy annihilation processes that could operate at room temperature. Our present results suggest that

the production of divacancies can compete with the recombination process. It has already been reported that positrons can detect $V_{C\text{-}Si}$ divacancies at 90 K in nitrogen-doped ($n = 5.4\times10^{17}$ cm^{-3}) 6*H*-SiC irradiated with 2-MeV electrons at 4 K.[11] This indicates that $V_{C\text{-}Si}$ divacancies can be produced at temperatures lower than 300 K even with 2-MeV electrons. It suggests that the probability to create $V_{C\text{-}Si}$ divacancies in 6*H*-SiC is high.

Furthermore, this work allows us to discuss the location of the $V_{C\text{-}Si}$ divacancy 0/+ ionization level in the 6*H*-SiC band gap. $V_{C\text{-}Si}$ divacancies have been detected in neutral charge states in crystals irradiated at high 12-MeV H^+ fluence. In these crystals, as it has been shown by EPR,[35] the Fermi level is located around the $-/0$ ionization level of V_{Si}. We have seen above that the $-/0$ ionization level of V_{Si} is 1.2 eV under the conduction band in 6*H*-SiC.[38] Consequently, it can be proposed that $V_{C\text{-}Si}$ divacancy 0/+ ionization level is located at least 1.2 eV under the conduction band of the 6*H*-SiC.

VI. NEGATIVE IONS

In this study, positron trapping at two types of negative ions $A^-_{300\,K}$ and $A^-_{15\,K}$ has been observed both in as-received and irradiated crystals. The type $A^-_{300\,K}$ is detected at all measurement temperatures up to 300 K in both as-received and as-irradiated crystals. It follows that $A^-_{300\,K}$ is negatively charged in all crystals even in the highest-fluence irradiated crystals for which the Fermi level has been found to be attached to the $-/0$ ionization level of V_{Si} [i.e., $E_C - E = 1.2$ eV or $E - E_V = 1.9$ eV (Ref. 38)]. Such a type of defect has also been detected by Polity, Huth, and Lausmann[11] in both as-grown *n*-type ($n = 5.4\times10^{17}$ cm^{-3}) nitrogen-doped 6*H*-SiC and after 2-MeV electron irradiation. According to these authors, the negative ions induced by 2-MeV electron irradiation survive up to 1740 K. They have tentatively been attributed to antisites. It is interesting to note that these negative ions are also detected in as-grown 6*H*-SiC crystals. Thus we can infer that they are related to defects that survive cooling after crystal growth at approximately 1800 °C. In 4*H*-SiC Si_C and C_{Si} antisites are expected to be produced according to the calculated values of their formation energy E_F. The values calculated by Torpo *et al.*[40] are about 4 eV for C_{Si} and Si_C antisites and are of the same order as that for the carbon vacancy. From calculations realized in 3*C*, 2*H*, and 4*H* polytypes the charge states of C_{Si} and Si_C are expected to be, respectively, neutral and positive in *n*-type crystals. In 3*C*-SiC, the relaxed antistructure pair constituted by neighboring C_{Si} and Si_C antisites is, however, expected to have negative ionization levels in the band gap.[41] The ionization energy for the relaxed antistructure pair 0/− level has been calculated at $E - E_V = 1.3$ eV.[41] More recently, Mattausch, Bockstedte, and Pankratov performed *ab initio* density-functional theory calculations of electrical and optical properties of different defects in SiC possessing carbon-carbon bonds.[42] Among all the possible configurations of these C-C defects, they proposed that the carbon-split interstitial-antisite complex ($C_{sp,C_{Si}\langle100\rangle}$) that is composed of two carbon atoms sharing a silicon site could be the well-known DII defect observed in the four major polytypes of SiC by photoluminescence.[43,44] The authors have calculated the $-/2-$ ionization level of the $C_{sp,C_{Si}\langle100\rangle}$ defect at $E - E_V = 1.5$ eV in 3*C*-SiC. They proposed that this defect can be formed via several steps, the first one being the transformation of V_{Si} in a V_C-C_{Si} complex. From the cited results it appears to be well established that different antisite complexes can exist in negative charge states in the *n*-type as-received crystal. The creation of such defects by 12-MeV H^+ irradiation can contribute to the trapping of positrons at the negative ions such as acceptors in 6*H*-SiC.

Let us discuss here the concentration of the negative ions after 12-MeV proton irradiation. The lifetime spectra decomposition leads to the conclusion that, at room temperature, positron trapping is saturated and can occur either at negative ions or at $V_{C\text{-}Si}$ divacancies. In these conditions, the trapping rate $K(A^-_{300\,K})/K(V_{C\text{-}Si})$ ratio is equal to the intensity ratio I_1/I_2 obtained from the lifetime spectra decomposition[31] at room temperature. The intensity ratio I_1/I_2 is 65/35 = 1.85 at low fluence and decreases up to 29/81 = 0.34 at the highest fluence. To obtain the $C(A^-_{300\,K})/C(V_{C\text{-}Si})$ concentration ratio of the two defects, it is necessary to know the value of the trapping coefficients of the $V_{C\text{-}Si}$ divacancy and of the negative ion. For the trapping coefficient at the neutral $V_{C\text{-}Si}$ divacancy, we assume that it is of the same order as the value of trapping coefficient for the neutral divacancy in Si (μ_2^0). At 15 K, the value $\mu_2^0(15\,K) = 1.14\times10^{15}$ at. s^{-1} can be estimated from the experimentally determined trapping coefficient at the negatively charged Si divacancy in Si, $\mu_2^-(15\,K) = 4\times10^{16}$ at. s^{-1} (Ref. 45) and from the theoretically calculations,[33] giving the trapping coefficient ratio between neutral and negatively charged vacancies $\mu_V^0/\mu_V^- = 1/35$. Taking into account the fact that the trapping coefficient for the neutral vacancy defect is constant as a function of temperature,[33] we use $\mu_{V_{C\text{-}Si}}(300\,K) = 1.14\times10^{15}$ at. s^{-1} for the $V_{C\text{-}Si}$ divacancy trapping coefficient at 300 K in 6*H*-SiC. Concerning the negative ions, a trapping coefficient of 6.9×10^{16} s^{-1} has been estimated in electron-irradiated *n*-type 6*H*-SiC at 25 K by Polity Huth, and Lausmann.[11] Considering the theoretical temperature dependence of the trapping coefficient for negative ions,[34] $\mu_{A^-_{300\,K}}$ can be estimated at the value of approximately 1×10^{16} s^{-1} at 300 K. It follows that the concentration ratio $C(A^-_{300\,K})/C(V_{C\text{-}Si})$ can be estimated to be the I_1/I_2 ratio divided by a factor $\mu_{V_{C\text{-}Si}}/\mu_{A^-_{300\,K}}$ approximately equal to 10. The ratio $C(A^-_{300\,K})/C(V_{C\text{-}Si})$ varies with the proton fluence in the range from 0.18 estimated for the lowest fluence of 4×10^{14} H^+ cm^{-2} to 0.03 estimated for the highest fluence of 7.8×10^{16} H^+ cm^{-2}. Given the value of $V_{C\text{-}Si}$ concentration estimated above (Sec. V), the negative-ion concentration is expected to be of the order of 3×10^{17} cm^{-3} in 7.8×10^{16} H^+ cm^{-2} irradiated 6*H*-SiC crystal.

In addition to $A^-_{300\,K}$, another type of ion acceptor is detected in 6*H*-SiC: the $A^-_{15\,K}$ negative ions. These $A^-_{15\,K}$ negative ions have been observed only at low temperature as-received and proton-irradiated 6*H*-SiC. When proton fluence

becomes equal or higher than 4×10^{16} H^+ cm^{-2}, these traps are no longer detected by positrons. It means that their trapping rate becomes too low at this high proton fluence compared to the trapping rate at the other dominating defects, $A^-_{300\,K}$ and $V_{Si\text{-}C}$. The decrease of the trapping rate at the $A^-_{15\,K}$ defects with increasing proton fluence can indicate an effect of the Fermi level position either on the ion charge state or on their introduction rate.

VII. CONCLUSIONS

We have applied positron-annihilation spectroscopy to study vacancies in as-grown and 12-MeV proton-irradiated Al- or N-doped 6*H*-SiC crystals. We can infer from the temperature dependence of the lifetime spectra decomposition that neutral and negatively charged vacancy defects exist in doped 6*H*-SiC crystals before and after proton irradiation. The (202 ± 8)-ps lifetime corresponding to one type of vacancy defect is detected at low temperature in as-received *n*-type nitrogen-doped 6*H*-SiC. Another characteristic lifetime of 226 ± 5 ps is measured at room temperature in all the proton-irradiated nitrogen-doped 6*H*-SiC crystals. By comparison with earlier experimental and theoretical results, we associated the value 202 ± 8 ps with positron lifetime for the negatively charged V_{Si} silicon monovacancy and the value 225 ± 2 ps with positron lifetime for the neutral Si-C divacancy. In addition, different types of ionic acceptors are detected. One of them acts as strong trapping centers even at room temperature in as-received Al- or N-doped 6*H*-SiC crystals.

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[1] G. Pensl and W. J. Choyke, Physica B **185**, 264 (1993).
[2] T. Dalibor, G. Pensl, H. Matsunami, T. Kimoto, W. J. Choyke, A. Schöner, and N. Nordell, Phys. Status Solidi **162**, 199 (1997).
[3] M. O. Aboelfotoh and J. P. Doyle, Phys. Rev. B **59**, 10 823 (1999).
[4] L. A. de S. Balona and J. H. Loubser, J. Phys. C **3**, 2344 (1970).
[5] H. Itoh, N. Hayekawa, I. Nashiyama, and E. Sakuma, J. Appl. Phys. **66**, 4529 (1989).
[6] A. Rempel and H.-E. Schaefer, Appl. Phys. A: Mater. Sci. Process. **61**, 51 (1995).
[7] W. Puff, P. Mascher, A. G. Balogh, and H. Baumann, Mater. Sci. Forum **258–63**, 733 (1997).
[8] A. Kawasuso, H. Itoh, T. Ohshima, K. Abe, and S. Okada, J. Appl. Phys. **82**, 3232 (1997).
[9] S. Dannefaer, Appl. Phys. A: Mater. Sci. Process. **61**, 59 (1995).
[10] G. Brauer, W. Anwand, P. G. Coleman, A. P. Knights, F. Plazaola, Y. Picaud, W. Skorupa, J. Störmer, and P. Willutzki, Phys. Rev. B **54**, 3084 (1996).
[11] A. Polity, S. Huth, and M. Lausmann, Phys. Rev. B **59**, 10 603 (1999).
[12] C. C. Ling, A. H. Deng, S. Fung, and C. D. Beling, Appl. Phys. A: Mater. Sci. Process. **70**, 33 (2000).
[13] A. Kawasuso, F. Redmann, R. Krause-Rehberg, T. Frank, M. Weidner, G. Pensl, P. Sperr, and H. Itoh, J. Appl. Phys. **90**, 3377 (2001).
[14] M.-F. Barthe, L. Henry, C. Corbel, G. Blondiaux, K. Saarinen, P. Hautojärvi, E. Hugonnard, L. Di Cioccio, F. Letertre, and B. Ghyselen, Phys. Rev. B **62**, 16 638 (2000).
[15] D. T. Britton, M.-F. Barthe, C. Corbel, A. Hempel, L. Henry, P. Desgardin, W. Bauer-Kugelmann, G. Kögel, P. Sperr, and W. Triftshäuser, Appl. Phys. Lett. **78**, 1234 (2001).
[16] N. Achtziger, J. Grillenberger, and W. Witthuhn, Appl. Phys. Lett. **73**, 945 (1998).
[17] A. M. Strel'chuk, A. A. Lebedev, V. V. Kozlovski, N. S. Savkina, D. V. Davydov, V. V. Solov'ev, and M. G. Rastegaeva, Nucl. Instrum. Methods Phys. Res. B **147**, 74 (1999).
[18] M. Bruel, Electron. Lett. **31**, 1201 (1995).
[19] L. Di Cioccio, Y. Le Tiec, C. Jaussaud, E. Hugonnard-Gruyère, and M. Bruel, Mater. Sci. Forum **264**, 765 (1998).
[20] K. Saarinen, P. Hautojärvi, and C. Corbel, in *Identification of Defects in Semiconductors*, edited by M. Stavola (Academic, New York, 1998), p. 209.
[21] R. Krause-Rehberg and H. S. Leipner, *Positron Annihilation in Semiconductors* (Springer, Heidelberg, 1999).
[22] J. F. Ziegler and J. P. Biersack, *The Stopping and Range of Ions in Solids* (Pergamon, New York, 1985).
[23] J. M. Perlado, L. Malerba, A. Sanchez-Rubio, *et al.*, J. Nucl. Mater. **276**, 235 (2000).
[24] G. Brauer, W. Anwand, E.-M. Nicht, J. Kuriplach, M. Sob, N. Wagner, P. G. Coleman, M. J. Puska, and T. Korhonen, Phys. Rev. B **54**, 2512 (1996).
[25] T. Staab, L. M. Torpo, M. J. Puska, and R. M. Nieminen, Mater. Sci. Forum **353–356**, 533 (2001).
[26] C. C. Ling, C. D. Beling, and S. Fung, Phys. Rev. B **62**, 8016 (2000).
[27] A. Kawasuso, H. Itoh, S. Okada, and H. Okumura, J. Appl. Phys. **80**, 5639 (1996).
[28] A. Kawasuso, H. Itoh, T. Ohshima, K. Abe, and S. Okada, J. Appl. Phys. **82**, 3232 (1997).
[29] A. Kawasuso, R. Redmann, R. Krause-Rehberg, M. Yoshikawa, K. Kojima, and H. Itoh, Phys. Status Solidi B **223**, R8 (2001).
[30] M. Gong, S. Fung, C. D. Beling, and Z. You, J. Appl. Phys. **85**, 7604 (1999).
[31] C. Corbel and P. Hautojärvi, in *Positron Spectroscopy of Solids*, edited by A. Dupasquier and A. P. Mills Jr. (IOS, Amsterdam, 1995), p. 533.
[32] M.-F. Barthe, L. Henry, C. Corbel, and G. Blondiaux (unpublished).
[33] M. J. Puska, C. Corbel, and R. Nieminen, Phys. Rev. B **41**, 9980 (1990).
[34] C. Corbel, F. Pierre, K. Saarinen, P. Hautojärvi, and P. Moser, Phys. Rev. B **45**, 3386 (1992).
[35] H. J. von Bardeleben, J. L. Cantin, I. Vickridge, and G. Battistig, Phys. Rev. B **62**, 10 126 (2000).

[36] L. Torpo, M. Marlo, T. E. M. Staab, and R. M. Nieminen, J. Phys.: Condens. Matter **13**, 6203 (2001).
[37] M. A. Müller, A. A. Rempel, K. Reichle, W. Sprengel, J. Major, and H.-E. Schaefer, Mater. Sci. Forum **363–365**, 70 (2001).
[38] S. Arpiainen, K. Saarinen, P. Hautojärvi, L. Henry, M.-F. Barthe, and C. Corbel, Phys. Rev. B **66**, 075206 (2002).
[39] W. Puff, A. G. Balogh, P. Mascher, and H. Baumann, Mater. Sci. Forum **248–249**, 285 (1997).
[40] L. Torpo, M. Marlo, T. E. M. Staab, and R. M. Nieminen, J. Phys.: Condens. Matter **13**, 6203 (2001).
[41] L. Torpo and R. M. Nieminen, Mater. Sci. Eng., B **61–62**, 593 (1999).
[42] A. Mattausch, M. Bockstedte, and O. Pankratov, Physica B **308–310**, 656 (2001).
[43] L. Patrick and W. J. Choyke, J. Phys. Chem. Solids **34**, 565 (1973).
[44] S. G. Sridhara, F. H. C. Carlsson, J. P. Bergman, A. Henry, and E. Janzen, Mater. Sci. Forum **353–356**, 377 (2001).
[45] P. Mascher, S. Dannefaer, and D. Kerr, Phys. Rev. B **40**, 11 764 (1989).