

## **Intrinsic Defects**

### **The Nature and Diffusion of Intrinsic Point Defects (Invited) in SiC**

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### **C-Interstitials in SiC: a Model for the DII Center**

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### **Radiation-Induced Defects in 4H and 6H SiC Epilayers Studied by Positron Annihilation and Deep Level Transient Spectroscopy**

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### **Chemical Environment of Atomic Vacancies in Electron Irradiated Silicon Carbide Measured by Two-Detector Doppler Broadening Technique**

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### **Vacancy Defects in as Polished and High Fluence H<sup>+</sup> Implanted 6H-SiC Detected by Slow Positron Annihilation**

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### **ESR Characterization of SiC Bulk Crystals and SiO<sub>2</sub>/SiC Interface**

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### **EPR Study on the Single Silicon Vacancy Related Defects in 4H-, 6H-SiC N.**

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### **Electrical Activation of Implanted Phosphorus Ions (Late News) in (0001)/(112 – 0)-Oriented 4H-SiC**

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### The nature and diffusion of intrinsic point defects in SiC

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In SiC intrinsic point defects inevitably occur. Incorporated during growth or induced by processing they can reduce the electronic quality of the material. In addition mobile intrinsic defects, namely vacancies and interstitials, play a pivotal role in the annealing kinetics and mass transport. For example in recent experiments [1] a transient enhanced dopant diffusion was observed that seriously affected the implanted dopant profiles. An analysis of diffusion profiles [2] indicates that most likely silicon interstitials drive the boron migration in SiC. However, any question related to the mechanisms of defect migration at the same time addresses the nature of the involved defects.

Based on an *ab initio* method we have developed a microscopic theory of the mobile intrinsic defects and their migration. The investigation of the ground state properties of interstitials, vacancies, antisites and their complexes forms the basis of our study. The calculation of hyperfine parameters and localised vibrational modes enables us to contribute to the identification of experimentally observed defect centers.

Our investigation of the defect hierarchy shows that silicon interstitials and carbon vacancies are the most abundant mobile intrinsic defects in p-type and intrinsic material. The latter also dominate under n-type conditions. Silicon vacancies, which in n-type material dominate over silicon interstitials, play a special role. Our calculation reveal that the vacancy is a metastable/bistable defect (3C-SiC and 4H-SiC resp.) that can transform into a carbon-vacancy-antisite-complex. In p-type material this transformation is accompanied with a large energy gain. Therefore we find that silicon interstitials are the only mobile Si-related defects under these conditions. However, in n-type material we expect a relevant contribution from the vacancy to diffusion as its migration on the Si-sublattice has a lower barrier than the above mentioned transformation. The migration of carbon vacancies proceeds entirely on the carbon sublattice. According to our calculations they are rather immobile which is in contrast to the high mobility deduced from the annealing behaviour of the EPR-centers T5 [3] (3C-SiC) and EI5 [4] (4H-SiC) interpreted as carbon vacancies. Though our calculated hyperfine parameters do not support the assignment for the T5 center our results in 4H-SiC point to a correct interpretation of the latter. An explanation for the annealing behaviour is the recombination of the vacancy with carbon split-interstitials: their high mobility should be responsible for the observed effect. Another footprint of the mobile split interstitials is the D<sub>II</sub> photoluminescence center which is kinetically formed during the annealing. We identify this center as a complex formed by a carbon antisite and a carbon split-interstitial. The calculated localised vibrational modes nicely agree with the experimentally observed phonon replica [5]. We discuss in detail the nature of the relevant intrinsic defects and the impact of our findings on the dopant and self diffusion.

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### C-Interstitials in SiC: a Model for the D<sub>II</sub> Center

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For decades the microscopic structure of the D<sub>I</sub> and the D<sub>II</sub> centers in SiC has been subject to thorough investigations. Both centers occur independently of the polytype and the implanted dopant which has led to the assumption that they are intrinsic defects. While the structure of the D<sub>I</sub> center still remains uncertain, a C-di-interstitial configuration has been proposed for the D<sub>II</sub> center to explain the results of photo luminescence experiments [1,2]. The characteristic spectra show five one-phonon lines related to diamond-like localized vibrational modes (LVM) above the SiC bulk phonon spectrum and two localized modes within the SiC phonon gap (gap modes). The spectra persist annealing above 1700°C. A strong binding between the C-di-interstitial and its carbon bonds would qualitatively account for the observed thermal stability of the spectrum and the diamond-like LVMs. Employing a density functional theory based *ab initio* method we have analyzed the phonon modes of relevant defects with diamond-like bonding in the polytypes 3C and 4H. For the di-interstitial configuration we find a high formation energy of approximately 12 eV. Energetically much more favorable are split-interstitial configurations, i.e. two C-atoms sharing a lattice site [3], which are natural candidates for the D<sub>II</sub> center due to their C-dimer bond. The highly abundant carbon antisite is expected to be a thermally stable defect as well. It has much weaker carbon bonds, though, and hence cannot explain the observed high frequency LVMs. For a C-split-interstitial on an antisite (C<sub>spC<sub>Si(100)</sub></sub>) we find the diamond-like localized phonon modes in good agreement with the experiment. Additionally we are able to reproduce the two gap modes within the phonon band gap. The interstitial C<sub>spC<sub>Si(100)</sub></sub> is formed during the diffusion of the most abundant C-interstitial C<sub>sp(100)</sub> in a reaction with a carbon antisite. The latter C-interstitial has the lowest migration barrier among the intrinsic interstitials and vacancies [4] and its mobility is most likely responsible for the annealing of the carbon vacancy by an interstitial-vacancy recombination. From the large binding energy of C<sub>spC<sub>Si(100)</sub></sub> (3.7 eV–4.5 eV) we expect a high thermal stability of this defect, which parallels the properties of the D<sub>II</sub> center. We discuss in detail the relevance of C<sub>spC<sub>Si(100)</sub></sub> and the other defects as a model of the D<sub>II</sub> center.

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## Radiation-Induced Defects in 4H and 6H SiC Epilayers Studied by Positron Annihilation and Deep Level Transient Spectroscopy

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The understanding of fundamental properties of point defects in SiC is the key for device processing because the electronic characteristics of crystals are strongly altered by them. In this study, we characterized vacancy-type defects in 4H and 6H SiC epilayers induced by electron irradiation using positron annihilation and deep level transient spectroscopy (DLTS). From the correlation between positron annihilation and DLTS data using the same wafers, it is confirmed that complexes including silicon vacancies are the origin of the  $E_{1/2}$  levels in 6H SiC and the  $Z_{1/2}$  level in 4H SiC.

Specimens are chemical-vapor-deposition (CVD) grown *n*-type 4H and 6H SiC epilayers (5 μm thick) doped with nitrogen (the net donor concentration is  $5 \times 10^{15} \text{ cm}^{-3}$ ). These specimens were irradiated with 2 MeV electrons with doses from  $1 \times 10^{15}$  to  $3 \times 10^{17} \text{ e}^-/\text{cm}^2$  at room temperature. Isochronal annealing was conducted from 100 to 1700 °C for 30 min in vacuum or dry argon ambient. Positron annihilation (the Doppler broadening and

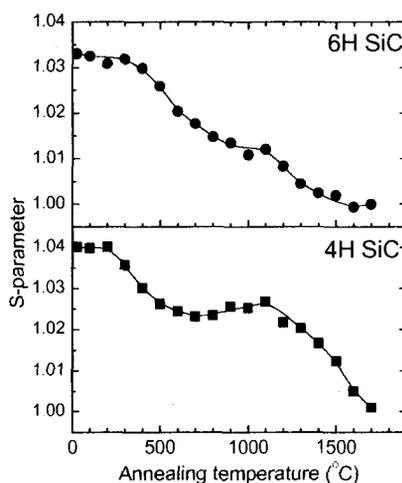


Fig. 1 Annealing behavior of *S*-parameters for the electron-irradiated 6H and 4H SiC specimens.

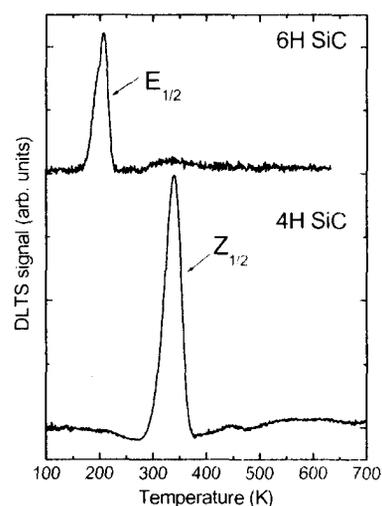


Fig. 2 DLTS spectra for the electron-irradiated 6H and 4H SiC specimens obtained after annealing at 1200°C.

lifetime) measurements were performed using slow positron beams at room temperature. After fabricating ohmic and Schottky contacts using Ni, DLTS measurements were carried out in the temperature range from 100 to 700 K.

Figure 1 shows the annealing behavior of the  $S$  parameter after electron irradiation (dose:  $3 \times 10^{17} \text{ e}^-/\text{cm}^2$ ). It is found that the  $S$  parameter decreases in two steps, i.e., until 600 °C and above 1000 °C in both polytypes. This shows that vacancy-type defects disappear in these temperature regions. The further analyses using the  $S$ - $W$  correlation and the coincidence Doppler broadening method shows that silicon vacancy-related defects dominate the above annealing processes [1]. Since isolated silicon vacancies are mobile below 1000 °C, the lower annealing stage can be attributed to the disappearance of isolated silicon vacancies and the other types of vacancies. The higher annealing stage should be interpreted in terms of complexes including silicon vacancies. From the DLTS measurements [2,3], a series of deep levels are found to be introduced in the upper half of the band gap. From Fig. 2, it is seen that the  $E_{1/2}$  level in 6H SiC and the  $Z_{1/2}$  level in 4H SiC, which are thought to have the same atomic arrangement in these polytypes, survive after annealing above 1000 °C. Consequently, these levels should be compared with the vacancy-type defects detected by positron annihilation. As shown in Figs. 3(a) and (b), the positron trapping rate (proportional to the defect concentration) of silicon vacancy related complexes and the concentration of the corresponding DLTS centers decreases in the similar way during the annealing between 1000 and 1500 °C. This allows us to conclude that the  $E_{1/2}$  and  $Z_{1/2}$  level in 6H and 4H SiC, respectively, are related to complexes including silicon vacancies.

[1] A. Kawasuso *et al.*, JAP to be published.

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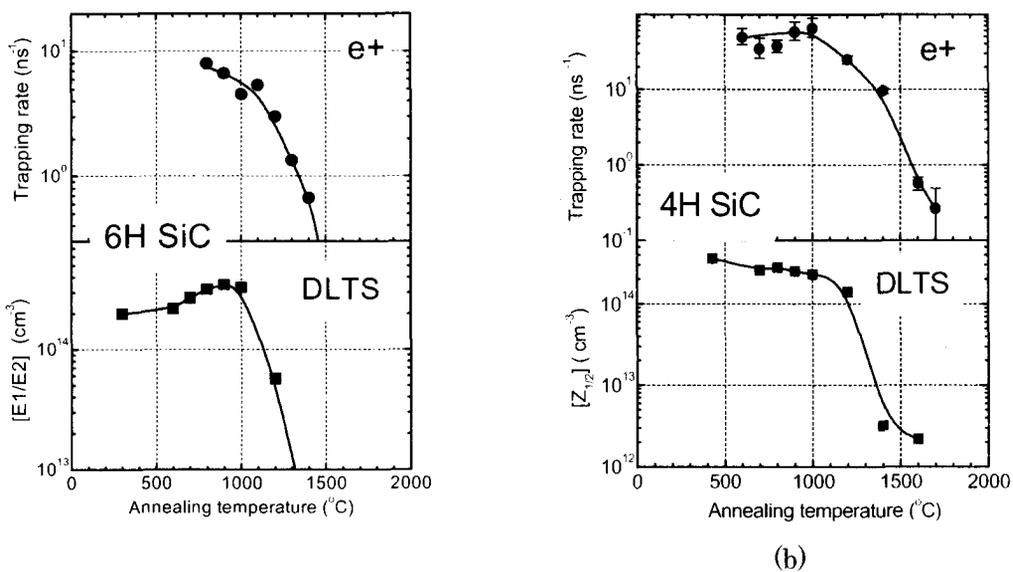


Fig. 3 Comparison between the positron trapping rate related to silicon vacancies and the concentrations of (a)  $E_{1/2}$  levels in 6H and (b)  $Z_{1/2}$  levels in 4H specimens.

## Chemical environment of atomic vacancies in electron irradiated silicon carbide measured by a two-detector Doppler broadening technique

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The paper presents a new positron annihilation technique [1] for the characterization of lattice defects in 6H-SiC in combination with the generation of defects by electron irradiation. The two-detector (2D) Doppler broadening technique allows the determination of the chemical environment of lattice defects which trap positrons. Coincident measurement of the energy of the two positron-electron annihilation photons gives the possibility to increase the signal to noise ratio up to  $10^5$  and extends the range of measurements of a Doppler broadened line up to  $(511 \pm 15)$  keV. The high energy part of the Doppler broadened spectrum is characteristic for the carbon and silicon core electron momentum distribution and therefore contains information about the chemical environment of a lattice defect in SiC.

For the present studies single crystals of 6H-SiC (Cree Inc., Durham, NC, USA) with n-type conductivity were used. Coincident measurements of the Doppler broadening of the positron-electron annihilation  $\gamma$  spectrum for background suppression were performed with a collinear set-up of two high-purity Ge detectors. The full-width at half-maximum (FWHM) of the energy resolution function was equal to about 1.2 keV. The positron lifetime was measured by means of a fast-slow  $\gamma\gamma$  spectrometer with a time resolution of 205 ps (FWHM). For both techniques a  $^{22}\text{NaCl}$  positron emitter stacked between two identical SiC specimen plates was used. The irradiation experiments on 6H-SiC for the generation of vacancies on both carbon and silicon sublattices by electrons of the energies: 0.5, 1, and 2 MeV and doses of about  $10^{-23} \text{ m}^{-2}$ , were performed at the Dynamitron accelerator of Stuttgart University.

The ratios of the coincident counts of the Doppler broadening measured for the electron irradiated SiC and for the reference materials are plotted in Fig.1. As determined by the model suggested in [2] and applied in [3] for 6H-SiC the electron momentum range lower than  $20 m_0c \cdot 10^{-3}$  is due to annihilation of the positrons with valence electrons. Because of the low number of counts the range above  $40 m_0c \cdot 10^{-3}$  is strongly affected by the background and all ratio curves independent of specimen meet there at the value of one (see Fig.1). Therefore, to obtain information about the chemical environment of the positron annihilation site in SiC only the shape of the ratio curves in the range from 20 to  $40 m_0c \cdot 10^{-3}$  (see Fig.1) is considered. The position of the whole ratio curves with respect to the ordinate is proportional to the intensity of the core electron component or to the density of the material in the positron annihilation site and is independent from the chemical environment of this site.

In the range from 20 to  $40 m_0c \cdot 10^{-3}$  the characteristic behavior of carbon core electrons shows a positive slope and that of silicon core electrons a negative slope of the ratio curve as obtained from the measurements on diamond and Si single crystals respectively (see Fig.1). The opposite slope of the ratio curves for carbon and silicon originates from positron annihilation with core electrons of both carbon and silicon atoms in as-grown SiC. The sum of two linear curves with opposite slope gives a horizontal line for as-grown SiC. The

delocalized positron wave function in this specimen overlaps the electron wave functions of both carbon and silicon core electrons and positrons are annihilated from the free state. The measured positron lifetime of 148 ps is close to the calculated free positron lifetime for SiC and supports this result.

The ratio curves for SiC irradiated by 1 MeV (Fig.1) and by 2 MeV electrons have positive slopes which are characteristic for carbon core electrons and therefore positrons are trapped by silicon vacancies in these specimens. The much lower position of the curve in comparison to non-irradiated carbide reflects the smaller overlap of the positron wave function with core electrons of atoms around the free volume of the vacancy. The positron lifetime of 210 ps measured for both of these specimens can be attributed to the silicon vacancy. The ratio curve for SiC irradiated by 0.5 MeV electrons has an intermediate position and almost no slope (Fig.1). Therefore, positrons are annihilated with core electrons of both carbon and silicon atoms in this specimen. This is in agreement with the positron lifetime of 179 ps which lies in between the silicon (210 ps) and the carbon (160 ps) vacancy positron lifetime. Therefore, the 0.5 MeV electrons displace nearly the same amount of C and Si atoms in SiC.

The present demonstration of the identification of vacancies on the two sublattices opens new potential for the attributing of energy levels in the band-gap of SiC to specific atomic defects.

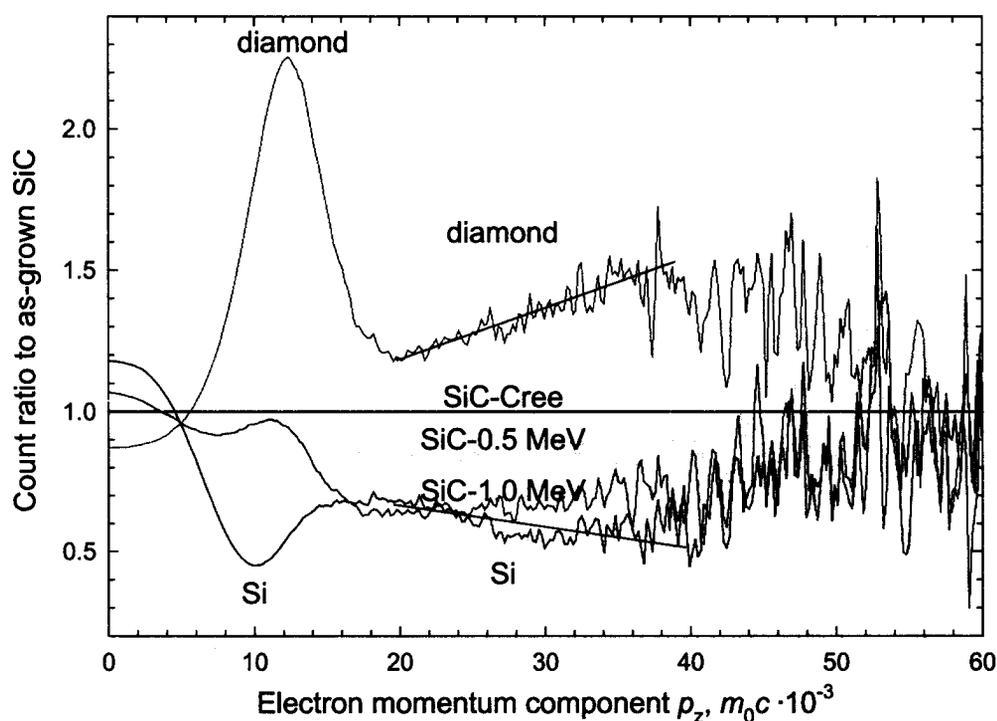


Fig.1. Count ratios of the 2D-Doppler broadened spectra of diamond, silicon, 6H-SiC after irradiation with 0.5 MeV and 6H-SiC after irradiation with 1.0 MeV electrons to the 2D-Doppler broadened spectrum of as-grown 6H-SiC. The lines for the diamond and Si single crystals curves are guides for the eye.

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## Vacancy defects in as-polished and in high fluence H<sup>+</sup> implanted 6H-SiC detected by slow positron annihilation spectroscopy

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Electronic and optoelectronic devices performances lies particularly on the surface and subsurface quality of the substrate used to build the structure. It is necessary to eliminate the defects generated by cutting process and surface preparation. Furthermore hydrogen implantation is used in SiC for passivation, doping and the Smart Cut process. However, the role and type of defects controlling the electrical properties in 6H-SiC(H) is far from fully understood.

Different characterization methods have been used to investigate the defects in semiconductors. Positron annihilation spectroscopy is a non destructive technique, which showed its power in detecting native and induced vacancy type defects in semiconductors. Slow positron beam based techniques allow to probe vacancy defects as a function of depth in the few  $\mu\text{m}$  range below the surface.

In this work we used slow positron annihilation spectroscopy to study on one hand the elimination of defects in as-polished bulk n-type 6H-SiC wafers and on the other hand the charge state of vacancy defects in high fluence H<sup>+</sup> implanted and annealed epitaxial n-type 6H-SiC layers.

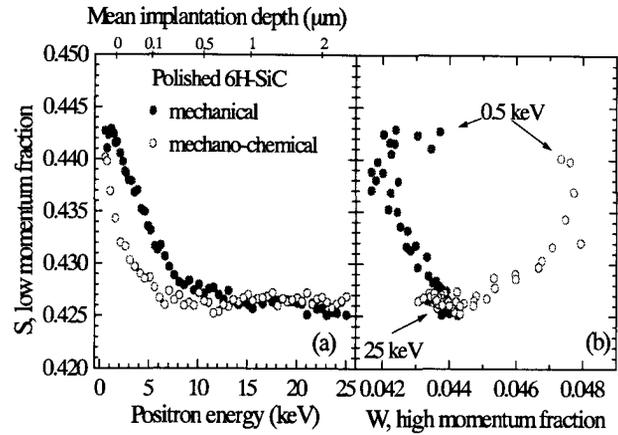
### I Defects investigated after polishing

The positron annihilation experiments were performed with a slow positron beam (ref 1) at the CERI laboratory in epitaxial and bulk n-type 6H-SiC wafers, in as-received state or after two different polish process performed by Novasic: a mechanical one and a mechano-chemical one.

The positron-electron pair momentum distribution has been investigated. It was measured at 300 K by recording the Doppler broadening of the 511 keV annihilation line which is proportional to the momentum component of the annihilating electron-positron pair,  $p_L$ , along the emission direction of the photons:  $2\Delta E_\gamma = cp_L$ . Two parameters are used to characterize the shape of the momentum distribution. The low momentum parameter S corresponds to the fraction of annihilations taking place in the momentum range  $(0-|2.80|) \times 10^{-3} m_0c$ . The high-momentum parameter W corresponds to the fraction of annihilations taking place in the momentum range  $(|10.61|-|26.35|) \times 10^{-3} m_0c$ . To investigate the depth dependence of S and W, the curves S(E) and W(E) were recorded as a function of the beam energy E changed

in 0.5 keV steps in the 0.5 to 25 keV range. The positron mean implantation depth in 6H-SiC varies from 5 nm to 2.1  $\mu\text{m}$  in this energy range.

S(E) and S(W) curves (Fig 1a and 1b) show that vacancy defects are present in the subsurface region in the only mechanically polished sample. These defects are not detected after the mechano-chemical polishing step.

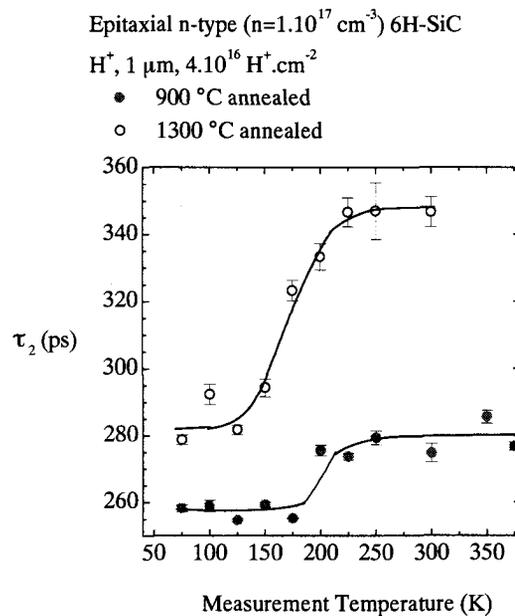


**Figure 1.** Low momentum fraction S as a function of positron beam energy (1a) and as a function of high momentum fraction W (1b) in 6H-SiC wafers polished in different conditions: only mechanical or mechano-chemical polishing .

## II Negatively charged vacancy defects in 6H-SiC after low energy H<sup>+</sup> implantation and annealing

The Smart Cut process is used to produce thin SOI heterostructures by low energy hydrogen implantation to fracture a thin layer after its bonding via SiO<sub>2</sub> to a SiO<sub>2</sub>/Si substrate. In highly doped n-type 6H-SiC, a partial compensation of the electrical activity persists after the 900°C annealing inducing the fracture.

We have used pulsed-slow-positron-beam-based positron lifetime spectroscopy to investigate the nature of acceptors and charge states of vacancy-type defects in low-energy proton-implanted 6H-SiC(H). We can infer from the temperature dependence of the lifetime spectra that neutral and negatively-charged vacancy clusters exist in the track region. Depending on annealing, they give rise to positron lifetimes of  $257 \pm 2$  ps,  $281 \pm 4$  ps and  $345 \pm 2$  ps, respectively. The 281 ps cluster has likely an ionization level near the middle of the bandgap. By comparison with theory, the 257 ps and 280 ps are identified as  $(V_C-V_{Si})_2$  and  $(V_C-V_{Si})_3$  clusters, respectively. In addition, other acceptors of ionic type act as strong trapping centers at low temperature ( $T < 150$  K). Neutral monovacancy-like complexes are also detected with a lifetime of  $160 \pm 2$  after 900° C annealing.



**Figure 2:** Long lifetime component extracted from positron lifetime spectra measured with 9keV positron as a function of temperature in H<sup>+</sup> ( $1 \mu\text{m}$ ,  $4.10^{16} \text{ cm}^{-2}$ ) implanted 6H-SiC after annealing at 900 and 1300°C.

## ESR characterization of SiC bulk crystals and SiO<sub>2</sub>/ SiC interface

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Impurities and defects, even in low concentrations, often strongly affect the electronic properties of device materials. At present, the process technology of SiC still remains at such a stage as one that requires a considerable refinement in controlling impurities and defects. Improvement of the doping efficiency is one of major subjects in the ion implantation doping. For the substrate crystals, lowering the concentration of unwanted impurities and defects are highly demanded. Reduction of the interface defects is important for improving the SiC-MOS device properties. ESR (electron spin resonance) is a powerful tool for identifying impurities and defects by supplying detailed microscopic structural information. Definite identification of point defects such as impurities, vacancies, anti-site-defects in various semiconductor crystals as well as interface defects (P<sub>b</sub> center) in SiO<sub>2</sub>/Si have been attained by using ESR. In our present work, we have applied ESR technique to characterize SiO<sub>2</sub>/SiC. Impurities and defects both in SiC substrate (i.e. bulk crystals) and at SiO<sub>2</sub>/SiC interface have been studied.

### 1. Dangling bond type defect

The identification of the P<sub>b</sub> center to be a silicon dangling bond at the silicon surface of the SiO<sub>2</sub>/Si(111) interface has been well-established. Searching of an ESR signal that is arising from an interface defect having a structure similar to the P<sub>b</sub> center has been, so far, failed in SiO<sub>2</sub>/SiC. In the samples of SiO<sub>2</sub>/p-6H-SiC(0001), we have found a new ESR spectrum (denoted here as PERC-1) that is arising from a silicon dangling bond along the [0001] axis. The carrier concentration of the substrate was  $\sim 1 \times 10^{14} \text{cm}^{-3}$ . The oxidation was performed at 1200°C in dry O<sub>2</sub>. As shown in Fig.1, the spectrum consists of a set of primary line and <sup>29</sup>Si (I=1/2, natural abundance 4.67%) hyperfine lines with B//[0001]. With the crystal rotated around [1100], the spectrum splits into two sets. We assume that the splitting is caused by site-splitting. The <sup>29</sup>Si hyperfine interaction determined by fitting of the angular dependence of the line positions is nearly axial with the three principal values 123.8, 123.9, and 172.2 G, respectively. The largest principal value is along [0001]. The wave function of the unpaired electron is described by the linear combination of atomic orbital approximation:

$$\Psi = \eta (\alpha \phi_{3s} + \beta \phi_{3p}) + \dots$$

The orbital parameters for the silicon atom giving the <sup>29</sup>Si hyperfine interaction are listed in

TABLE. We note that a high fraction ( $\eta^2=0.64$ ) of the unpaired electron is localized on one silicon atom with a high  $p$ -character ( $sp$  ratio:  $\beta^2/\alpha^2 = 4.6$ ). The direction of the  $p$ -orbital is along  $[0001]$ . Thus, the PERC-1 center has a dangling-bond character expected for  $P_b$ -like interface defect. The signal does not exhibit a strong anisotropy of the line width that is distinctly observed in the  $P_b$  center and that is caused by distribution of structure. To identify that the PERC-1 spectrum is arising not from such centers in the bulk as dangling bonds at void and vacancy-impurity complexes but from interface defects, the location of the center needs to be determined.

An ESR signal similar to PERC-1 has been observed also in  $\text{SiO}_2/4\text{H-SiC}$ . In the samples of  $\text{SO}_2/4\text{H-SiC}$ , there exists a dominantly strong isotropic signal. To extract selectively the relatively weak signal of the dangling bond center which is hidden underneath the strong isotropic signal, pulsed-ESR technique has been utilized.

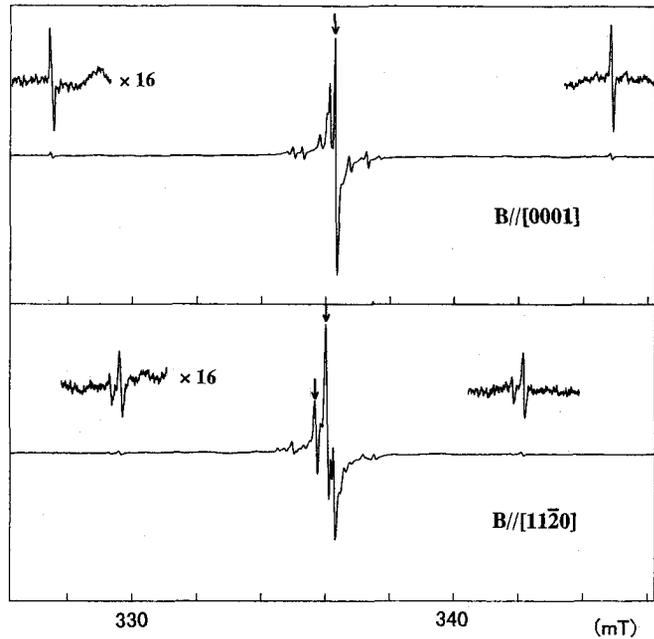
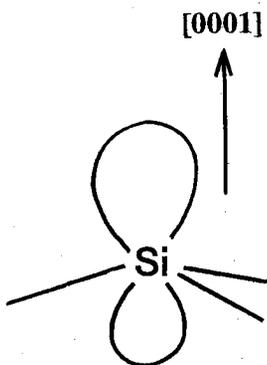


Fig.1 ESR spectrum of  $\text{SiO}_2/p\text{-6H-SiC}$  (R.T.)

TABLE. Hyperfine and orbital parameters

	$A_{//}/g_e\beta_e$ (G)	$A_{\perp}/g_e\beta_e$ (G)	$\alpha^2$	$\beta^2$	$\eta^2$
PERC-1	172	124	0.18	0.82	0.64
$P_b$ center <sup>1</sup>	156	91	0.12	0.88	0.80

<sup>1</sup>K. Brower, Appl. Phys. Lett. 43, 1111 (1983)

## 2. Impurities

As demonstrated in Fig.2, the samples of  $\text{SiO}_2/p\text{-6H-SiC}$  exhibit a relatively large number of signals of impurities and defects. Most of them are arising from the substrate. ESR parameters and the structural models of these impurities will be presented.

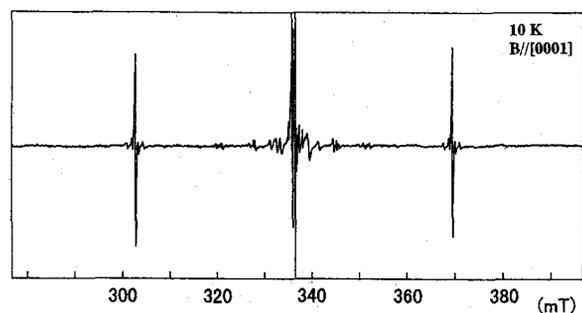


Fig.2 ESR spectrum of  $\text{SiO}_2/p\text{-6H-SiC}$

## EPR study on the single silicon vacancy related defects in 4H-, 6H-SiC

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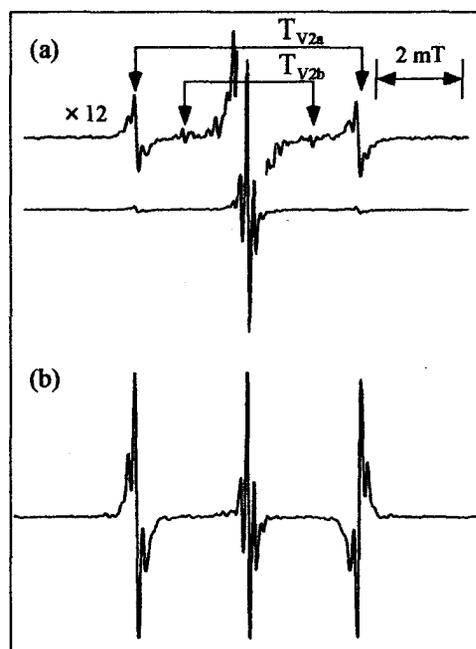
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The spin triplet ( $S=1$ ) single silicon vacancy related defects in electron irradiated n-type 4H, p-type 6H-SiC were studied by electron paramagnetic resonance (EPR) spectroscopy. By laser irradiation, the hyperfine couplings (HFC) with nearest-neighbor (NN) atoms of  $T_{V2a}$  were observed for the first time. From the detailed analysis,  $T_{V2a}$  was unambiguously assigned to be the single silicon vacancy.

Vacancy is one of the most important intrinsic defects. It exhibits interesting physics and is extensively studied experimentally and theoretically in many semiconductors. Particularly in SiC, it is well known that vacancy is stable even at room temperature (RT).

In our electron irradiation condition (3 MeV, total fluence  $4 \times 10^{18}$  e/cm<sup>2</sup> at RT), thermal equilibrated EPR signals of  $T_{V2a}$  and  $T_{V2b}$  in 4H-SiC were observed at RT for the first time as shown in figure 1 (a). In the previous optically detected magnetic resonance (ODMR) studies of  $T_{V2a}$  by E. Sörman et al.,<sup>1</sup> they observed small HFC that are very similar with those of the next-nearest-neighbor silicon of silicon vacancy. From this observation by ODMR, they suggested that  $T_{V2a}$  is the silicon vacancy related defect.<sup>1</sup>

For the assignment of the vacancy, it is important to know information of the NN atoms of the defect center. Furthermore, by obtaining the HFC constants of the NN atoms of the defect center, the detailed structural information can be obtained. For the detailed analysis of



Magnetic field

Fig. 1

HFC, the improvement of the signal to noise ratio is necessary because the natural abundances of the  $^{13}\text{C}$  (1.1 %) and  $^{29}\text{Si}$  (4.7 %) isotopes are very small. Furthermore the selective amplification of the signal is also important not to be superimposed by other signals. To amplify the signal selectively, we irradiated the continuous wave laser light (808 nm; a Coherent FAP-system with 10 W)

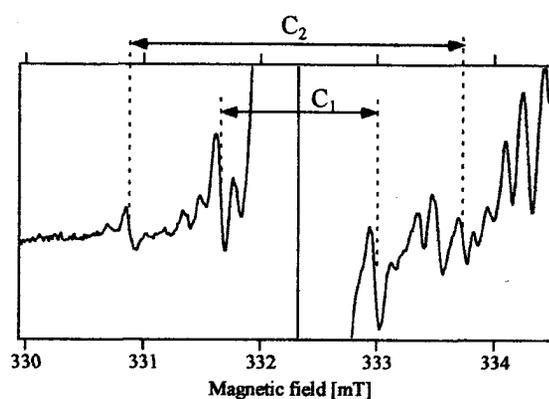


Fig. 2

during the X-band EPR measurement and could amplify the signal of  $T_{V2a}$  selectively as shown in figure 1(b). From this success, the HFC of NN atoms of  $T_{V2a}$  were observed for the first time and are shown as  $C_1$  and  $C_2$  in figure 2. The spectrum shown is the one when the magnetic field is parallel to the [0001] (c-axis). The intensity ratio between their total integrated intensity and that of the central line was 4.5 %. It almost corresponds to the theoretically calculated value (4.2 %) in the case that the NN atoms are four C atoms. None of the HFC of the common impurities in SiC, such as N, Al, B, Ti, V, or H, is observed. From these facts, it is revealed that the NN atoms around the  $T_{V2a}$  are four carbons.

We also investigated the angular dependence of the HFC of the NN. The obtained HFC constants are shown in Table. Obtained information from the analysis is summarized as follows. Its symmetry of the structure belongs to the  $C_{3v}$  point group. In the wavefunction of the unpaired electron, 57 % of the unpaired electrons is localized on the nearest four C atoms. From the observation of four  $^{13}\text{C}$  around  $T_{V2a}$  and the dense electron spin density on those,  $T_{V2a}$  can be unambiguously assigned to be the single silicon vacancy. From the estimated spin density and the very small D-value, it is considered that the extent of distortion along the c-axis is considered to be very small. The details of analysis and structural information will be presented.

TABLE. Hyperfine coupling constants ( $A_{iso}$ ; isotropic part,  $A_{aniso}$ ; anisotropic part)

	$A_{iso}$ (MHz)	$A_{aniso}$ (MHz)
A( $C_1$ )	44.8	15.5
A( $C_2$ )	50.0	15.1

<sup>1</sup>E. Sörman, N. T. Son, W. M. Chen, O. Kordina, C. Hallin, E. Janzén, *Phys. Rev. B* **61**, 2613 (2000).

**Electrical Activation of Implanted Phosphorus Ions in (0001)/(11 $\bar{2}$ 0)-oriented 4H-SiC**

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Rutherford Backscattering and Cross-Sectional Transmission Electron Microscopy investigations conducted by Satoh and Nakaike (1<sup>st</sup> Int. Workshop on Ultra-Low Loss Power Device Technology, May 2000, Nara, Japan) revealed that implantation-induced amorphous 6H-SiC epilayers oriented in (1 $\bar{1}$ 00)-direction could largely be recrystallized at 1500°C preserving the polytype of the underlying layer, while (0001)-oriented 6H-SiC epilayers showed a high density of extended defects even after an anneal at 1700°C.

In this study, we have performed comparative Hall effect investigations on phosphorus (P)-implanted, Si-face/a-plane ((0001)/(11 $\bar{2}$ 0)-oriented) p-type 4H-SiC epilayers in order to examine whether the electrical activation of P donors implanted into a-plane samples is also superior to that one in samples with Si-face. We implanted two P box profiles (profile 1:  $T_{impl} = \text{room temperature}$ , depth = 1.3  $\mu\text{m}$ ,  $[P] = 10^{18} \text{ cm}^{-3}$ , profile 2:  $T_{impl} = 500^\circ\text{C}$ , depth = 0.8  $\mu\text{m}$ ,  $[P] = 10^{20} \text{ cm}^{-3}$ ) and performed annealings in the temperature range from 1400° to 1700°C. As an example, the temperature dependence of the free electron concentration  $n$  and of the electron Hall mobility  $\mu$  for two pairs of samples oriented in (0001) (samples 1(Si)/2(Si)) and in (11 $\bar{2}$ 0) (samples 1(a)/2(a)) direction are displayed in Figs. 1(a)/(b). Sample 1/2 was implanted with the P profile 1/2. All the samples were annealed at 1600°C. The following results are observed: (i) The electrical activation of P donors implanted into (0001)- and (11 $\bar{2}$ 0)-oriented 4H-SiC epilayers is identical; the compensation in (0001)- oriented samples in general exceeds that one in (11 $\bar{2}$ 0)- oriented samples (see Fig. 1(a)). (ii) P donors can completely be activated in both types of samples up to a concentration of  $10^{20} \text{ cm}^{-3}$ . (iii) The electron Hall mobility strongly differs in (0001)/(11 $\bar{2}$ 0)-oriented 4H-SiC epilayers (see Fig. 1(b)); its ratio at room temperature is in samples #1:  $\mu(1(a))/\mu(1(\text{Si})) \approx 1.3$  and in samples #2:  $\mu(2(a))/\mu(2(\text{Si})) \approx 2.2$ . The physical reasons for the observed differences in the electron Hall mobility will be discussed in the paper.

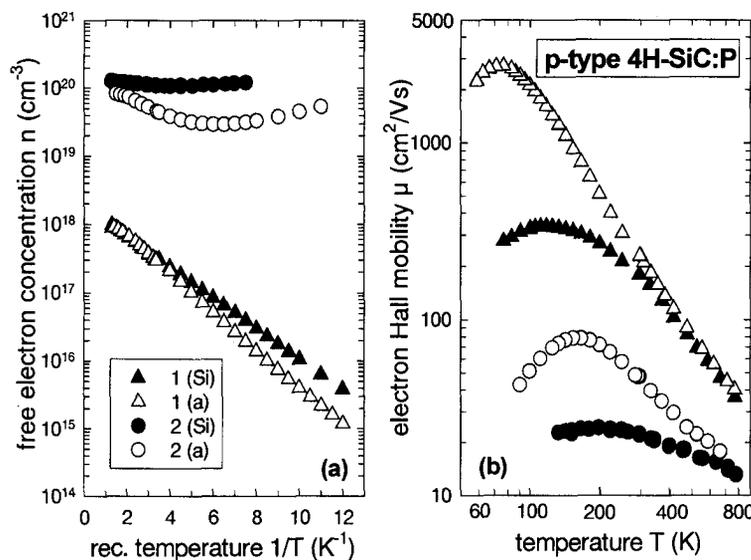


Fig.1: (a) Free electron concentration versus reciprocal temperature obtained from Hall effect investigations on P-implanted p-type 4H-SiC epilayers. (b) Hall mobility versus temperature.

Implantation:  
 samples 1(Si)/(a): P-box profile, depth = 1.3  $\mu\text{m}$ ,  $[P] = 10^{18} \text{ cm}^{-3}$ ,  $T_{impl} = \text{room temperature}$ .  
 samples 2(Si)/(a): P-box profile, depth = 0.8  $\mu\text{m}$ ,  $[P] = 10^{20} \text{ cm}^{-3}$ ,  $T_{impl} = 500^\circ\text{C}$ .  
 Annealing of samples 1(Si)/(a) and 2(Si)/(a):  
 $T_A = 1600^\circ\text{C}$ ,  $t_a = 30 \text{ min}$ .