

Interface Defects in n-type 3C-SiC/SiO₂: An EPR Study of Oxidized Porous Silicon Carbide Single Crystals

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Abstract. The defects at the 3C-SiC/SiO₂ interface have been studied by X-band EPR spectroscopy in oxidized porous 3C-SiC. One interface defect is detected; its spin Hamiltonian parameters, spin $S=1/2$, C_{3v} symmetry, $g_{\parallel}=2.00238$ and $g_{\perp}=2.00317$, central hyperfine interaction (CHF) with one carbon atom and $A_{B//[001]}=48\text{G}$ and superhyperfine (SHF) interaction with three equivalent Si neighbour atoms and $T_{B//[001]}=12.4\text{G}$, allow us to attribute the center to a sp^3 coordinated carbon dangling bond center, P_{bc}.

Introduction

The thermal oxidation of silicon carbide monocrystals has been intensively studied in the past due to the interesting differences as compared to the case of silicon and due to its technological importance for the formation of high quality metal oxide semiconductors (MOS) SiC/SiO₂ structures. Most of these studies have been performed on the 4H and 6H-SiC polytypes; the results have been reviewed in [1,2]. Surprisingly, the oxidation kinetics at the usually employed temperature of $\sim 1100^{\circ}\text{C}$ are very different for the Si and C (0001) surfaces with a strongly reduced oxide growth rate at the Si face [3]. Further, and contrary to the case of Si/SiO₂ the oxide formation region at the semiconductor/dielectric interface seems to be much wider than for Si/SiO₂ [4].

As concerns the defects at the interface, the situation is also more complicated than in the Si/SiO₂ case. In addition to deep midgap states, difficult to assess by DLTS due to the large bandgap of SiC, high concentrations ($\sim 10^{13}\text{cm}^{-2}\text{eV}^{-1}$) of interface defects have been detected near both band edges [4]. The microscopic structure of the various interface defects is still an open question, which impedes the development of efficient defect reduction procedures. In the case of 4H- and 6H-SiC polytypes very recently the microscopic structure of one interface defect has been obtained from EPR studies [5,6]. As in the case of Si the use of oxidized porous samples has turned out to be decisive for these EPR studies [7]. Previous investigations on 3C, 4H, 6H n-type bulk single crystals had given only limited information and in particular no interface defect had been evidenced [8].

As concerns 3C-SiC/SiO₂ the previous EPR studies had been performed on epitaxial SiC layers deposited on Si substrates [8,9]. In these studies two oxide related centers have been evidenced; they are characterized by isotropic g-factors of 2.0044 et 2.0029, respectively and peak to peak linewidth of $\sim 2\text{G}$. Based on the numerical value of the g-factor and the evolution of the defect concentration following heat treatments they were tentatively attributed to Si and C dangling bond centers in the amorphous SiO₂ layer. We report here the results of an EPR study of oxidized porous bulk SiC which reveal for the first time a paramagnetic interface defect in 3C-SiC/SiO₂.

Experimental details

The porous layers of $\sim 100\mu\text{m}$ thickness were formed by electrochemical dissolution of (100) oriented, polished n-type 3C-SiC bulk substrates. Typical sample dimensions were $2 \times 6\text{mm}^2$. They were oriented with [100] or [110] along the long axis. The samples were then oxidized in a clean furnace in dry oxygen at 1000°C under an oxygen pressure of 30mbar for 10min. The oxide thickness was estimated to be 1-2nm. The EPR measurements were performed with an X-band spectrometer (9.6GHz) at 300K. Angular variations of the EPR spectra for a rotation of the magnetic field in the (100) and (110) planes were recorded.

Experimental Results and Discussion

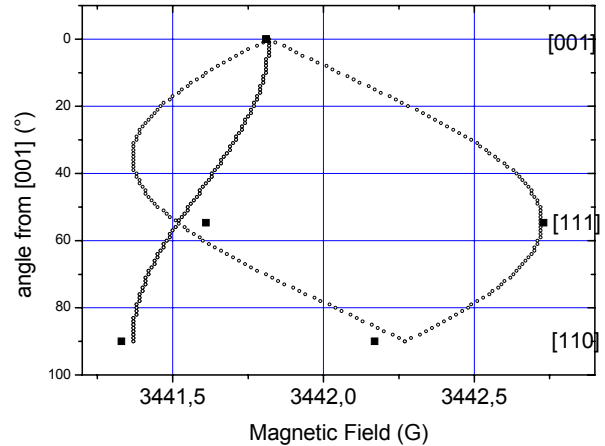
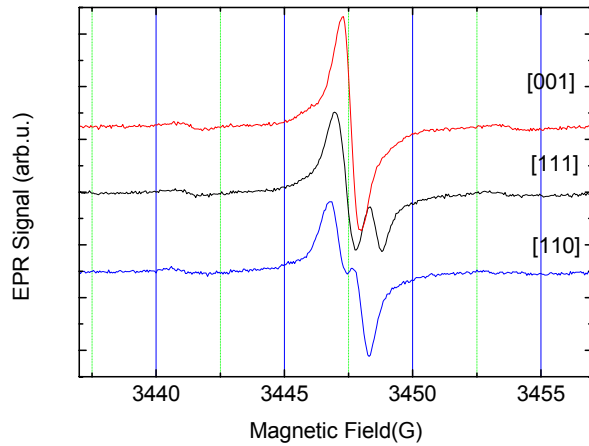


Fig.1 EPR spectra of oxidized porous 3C-SiC for three orientations of the magnetic field ; $T=300\text{K}$

Fig.2 Simulated angular dependence and experimental resonance fields; numerical values are given in table 1

After oxidation we observe one dominant anisotropic EPR spectrum with two resolved lines for a

Polytype, sample	g -tensor linewidth CHF constant SHF constant	sym.axis	model	reference
3C-bulk, porous	$g_{//}=2.00238$ $g_{\perp}=2.00317$ $\Delta B_{pp} \sim 0.6\text{G}$ CHF: $A_{//[001]}=48\text{G}$ SHF $T=12.4\text{G}$	[111]	Interface defect: [111] Carbon dangling bond center at the SiC interface P_{bc}	This work
4H-bulk, porous	$g_{//}=2.0023$ $g_C=2.0032$ $g_{xx}=2.0031$ $g_{yy}=2.0028$ $g_{zz}=2.0023$ $\Delta B_{pp} \sim 0.7\text{G}$ SHF $T=12.4\text{G}$	[0001] [11-20]	Interface defect P_{bc} ----- P_{bc}	[5,6]

Table 1: Comparison of P_{bc} center parameters in 3C and 4H-SiC

variation of the magnetic field in the (110) plane. Figure 1 shows a typical EPR spectrum taken at 300K for the three principal orientations of the magnetic field parallel to [001], [111] and [110]. The

spectrum can be decomposed into two lines of $\sim 0.6\text{G}$ peak-to-peak linewidth for $B//[111]$ and $B//[110]$.

For $B//[100]$ the spectrum collapses into one single line. Let us recall that the porous sample is a three dimensional structure in which all different surface orientations may exist. Thus, we may expect to find the four possible orientations of oxidized (111) surfaces, whereas in a bulk sample of course only the external surface will be developed. The surfaces in porous samples are related to the dissolution conditions and often high density surfaces such as (111) are predominantly developed. For an interface defect at (111) SiC/SiO_2 with axial symmetry we would thus expect four different defect orientations and the same number of EPR lines for a general orientation of the magnetic field. For the high symmetry planes (100) and (110) they will reduce to 2 and 3 branches respectively. The angular variation observed for a rotation in the (100) and (111) planes (fig.1,2) is characteristic for a [111] oriented axially symmetric defect. The angular variation can be well fitted with an [111] axial g-tensor with principal values of $g_{\parallel}=2.00238$ and $g_{\perp}=2.00317$.

As shown in fig.1 and in more detail in fig.3, the central lines are accompanied by low intensity hyperfine lines, which for $B//[001]$ have a splitting of 12.4G . At higher gain, in addition to these hyperfine lines an additional doublet with twice the splitting can be observed (fig.3), which demonstrates that the lines are due to the superhyperfine (SHF) interaction with ligand atoms. The intensity ratio of the SHF lines to the central line is $\sim 0.12 \pm 0.03$. If the linewidth of the central and SHF lines were the same, an amplitude ratio of 0.15 should be expected but due the slightly increased line width of the SHF lines requires a numerical integration for this evaluation. From this we attribute the SHF structure to an interaction with a three Si neighbour shell. This is the configuration of the 1st and 3rd nearest neighbour (NN) shells for a carbon site defect. A priori the assignment to the 1st NN shell seems to be most probable as the SHF interaction is decreasing with increasing neighbour distance but a theoretical study of the spin distribution of this center is required for a definite assignment.

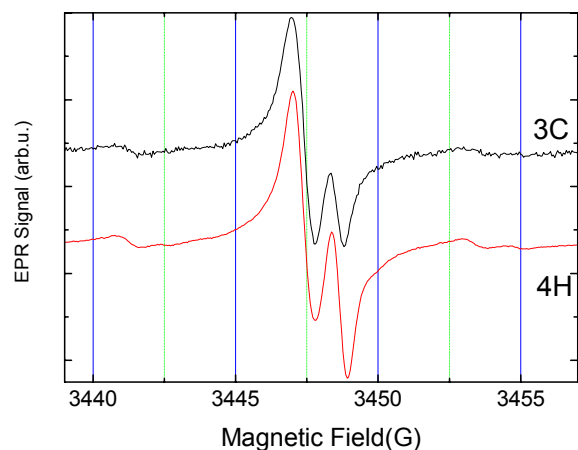
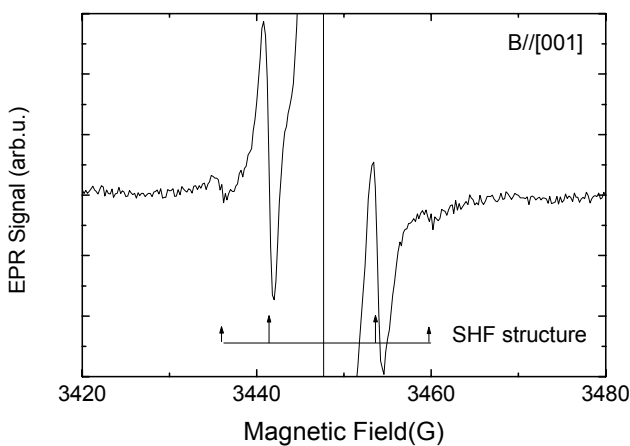


Fig.3 SHF structure of the P_{bC} center displaying lines from interaction with one ^{29}Si and two ^{29}Si atoms in a three atom NN neighbours shell

Fig.4 Comparison of the P_{bC} center EPR spectra in porous 3C- and 4H-SiC/SiO₂; $B//[111]$ and $B//[0001]$ respectively

The EPR parameters of this center are very close to the one's observed for the carbon P_{bC} center in 4H and 6H polytypes [4,5] and we attribute this center in agreement with the previous assignments to a carbon dangling bond defect at the SiC side of the SiC/SiO_2 interface.

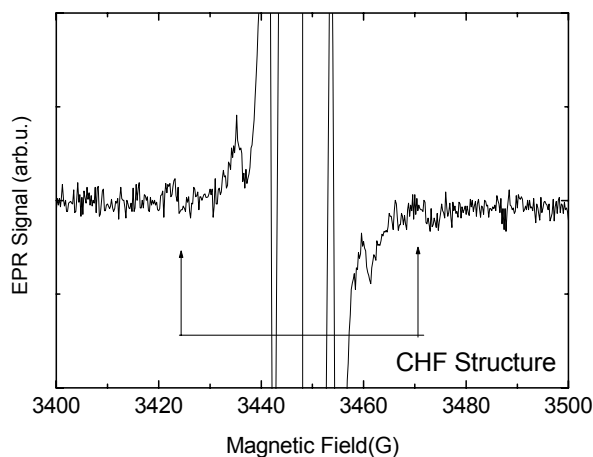


Fig.5 Central hyperfine structure doublet for $B//[001]$

A direct proof for the chemical nature of the central atom is the observation of the central hyperfine (CHF) interaction. In the case of carbon related defects this is always a difficult task in CW EPR due to the low isotopic abundance (1.1 %) of the only isotope with non zero nuclear spin ^{13}C ($I=1/2$). In addition, the higher linewidths of the HF lines of interface defects further reduce the amplitude ratio of the HF lines to the central lines. Nevertheless, for the most favourable orientation of the magnetic field $-B//[001]$ - for which all CHF lines are expected to coalesce into one doublet we do indeed observe a doublet with a HF constant of $A_{//[001]}= 48\text{G}$. The intensity ratio is

in good agreement with the one expected for a carbon dangling bond center, which confirms our assignment (fig.5). The angular dependence of the CHF structure has not yet been measured. We can compare the value of $A_{//[001]}$ measured here with the equivalent one in 4H-SiC/SiO₂. Assuming axial symmetry the values of [5] predict a value of $A=54\text{G}$ for an angle $(B,[0001])=54^\circ$ which once again is of the same order as the one in the 3C polytype.

Conclusion

We have observed by EPR spectroscopy in 3C-SiC/SiO₂ a (111) plane related defect which from its spin Hamiltonian parameters can be attributed to a carbon P_{bc} center. This defect has nearly identical parameters as those observed in the case of 4H and 6H polytypes. Such a similarity in g-values and HF interaction constants has previously been observed for numerous intrinsic defects 3C and 4H, 6H polytypes.

Acknowledgments

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