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Relationship between defects induced by irradiation and reduction of hole concentration in Al-doped 4H–SiC

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Abstract

From the temperature dependence of the hole concentration in lightly Al-doped 4H–SiC epilayers, a shallow acceptor with $E_V + 0.2 \text{ eV}$, which is an Al atom (Al_{Si}) at a Si sublattice site, and an unknown deep defect with $E_V + 0.35 \text{ eV}$ are found, where E_V is the valence band maximum. In unirradiated epilayers, moreover, the density (N_{Defect}) of this defect is close to the Al acceptor density (N_{Al}). With irradiation of 0.2 MeV electrons, the N_{Al} is reduced, while the N_{Defect} is increased. Judging from the minimum electron energy required to displace a substitutional C atom (C_s) or Al_{Si}, the bond between Al_{Si} and its nearest neighbor C_s is broken due to the displacement of the C_s by this irradiation. Moreover, the displacement of the C_s results in the creation of a complex (Al_{Si}-V_C) of Al_{Si} and its nearest neighbor C vacancy (V_C), indicating that the possible origin of the defect with $E_V + 0.35 \text{ eV}$ is Al_{Si}-V_C. \bigcirc 2005 Elsevier B.V. All rights reserved.

Keywords: Al-doped 4H-SiC; Electron irradiation; Radiation damage; Reduction in hole concentration

1. Introduction

Silicon carbide (SiC) is a promising wide band gap semiconductor for fabricating high-power and high-frequency electronic devices capable of operating at elevated temperatures.

From the temperature dependence of the hole concentration p(T) for lightly Al-doped 4H–SiC epilayers, one acceptor species with ~200 meV and one defect with ~350 meV are observed [1,2], where all the energy levels are measured from the valence band maximum (E_V). From photoluminescence (PL) [3], the acceptor species is ascribed to an Al atom (Al_{Si}) at a Si sublattice site. However, the origin of this defect has so far not been determined.

This defect cannot be determined accurately from deep level transient spectroscopy (DLTS), since the density (N_{Defect}) of this defect is nearly equal to the density (N_{Al}) of the Al acceptor. This is because DLTS can determine the energy levels and densities of defects only when the defect density is much lower than the acceptor density.

Irradiation with 4.6 MeV electrons at 2.6×10^{14} cm⁻² fluence reduced the N_{Al} by ~10, while reducing the N_{Defect} only slightly [2]. Therefore, the reduction in p(T) with this irradiation results from a decrease in N_{Al} due to the displacement of the Al_{Si} or the bond breaking between Al_{Si} and its nearest neighbor C.

Boron (B) in 4H–SiC was reported to form two electrical levels in the lower half of its bandgap [4]. One is located at \sim 300 meV as determined by Hall-effect measurements [4], and the other is between 550 and 650 meV as determined by DLTS [5]. The shallow level is assigned to a B atom (B_{Si}) at a Si sublattice site. The probable identification of the deep level is a complex (B_{Si}–V_C) of B_{Si} and its nearest neighbor C vacancy (V_C) [6,7].

By analogy with B in 4H–SiC, the deep defect in Aldoped 4H–SiC may be an $Al_{Si}-V_C$ complex, which was detected by electron paramagnetic resonance (EPR) spectroscopy [7].

Since the atomic mass of C is smaller than that of Si, the maximum energy transferred from one electron to one

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substitutional C atom (C_s) in SiC by elastic collision is larger than that to one substitutional Si atom (Si_s). This indicates that the minimum electron energy necessary for displacing one C_s should be lower than that for one Si_s .

In this article, we report on our investigation of the origin of the unknown deep defect as well as the mechanism for the reduction in N_{Al} by irradiation with electrons of several energies. The densities and energy levels of acceptors and defects are determined by free carrier concentration spectroscopy (FCCS) from the p(T) without any assumptions regarding the acceptor species and the defects.

2. Experiment

A 10 µm-thick lightly Al-doped p-type 4H-SiC epilayer on n-type 4H–SiC (thickness: $376 \,\mu\text{m}$, resistivity: $0.02 \,\Omega\text{cm}$) was cut to a $1 \times 1 \text{ cm}^2$ size. Ohmic metal (Ti/Al) was deposited on the four corners of the surface of the sample, and then the sample was annealed at 900 °C for 1 min in an Ar atmosphere. The p(T) and the temperature dependence of the hole mobility $\mu_n(T)$ were measured by van der Pauw configuration in the temperature range from 120 to 600 K in a magnetic field of 1.4T using a modified MMR Technologies' Hall system. The sample was irradiated with 1.0×10^{16} cm⁻² fluence of 0.2 MeV electrons, 5.0×10^{15} or $1.0 \times 10^{16} \text{ cm}^{-2}$ fluence of 0.5 MeV electrons, or $1.0 \times$ 10^{16} cm⁻² fluence of 1 MeV electrons at room temperature. After the irradiation, the p(T) and the $\mu_{\rm p}(T)$ were measured.

3. Results and discussion

Fig. 1 shows the experimental p(T) for the sample (\circ) before irradiation and the samples irradiated with the $1.0 \times$ 10^{16} cm⁻² fluence of 0.2 MeV electrons (\triangle) and the 5.0 × 10^{15} cm^{-2} fluence of 0.5 MeV electrons (×). The p(T) for the sample irradiated with the $2.6 \times 10^{14} \text{ cm}^{-2}$ fluence of 4.6 MeV electrons is also shown by \diamond , which was reported previously [2]. Each $\mu_{\rm p}(T)$ seemed unchanged by the irradiation, indicating that the band conduction of holes is dominant in the temperature range of the measurement.

The p(T) for the sample irradiated with the 1.0 \times 10^{16} cm^{-2} fluence of 0.5 or 1 MeV electrons could not be measured, because of much higher resistivity of the sample. Since the p(T) for 10- Ω cm B-doped Si (B-doping density: $2 \times 10^{15} \text{ cm}^{-3}$) is reported to be reduced slightly by irradiation with 1.0×10^{16} cm⁻² fluence of 1 MeV electrons [8], the Al-doped p-type 4H-SiC is found to be less radiation resistant compared with B-doped Si, although it is generally accepted that SiC has a very high resistance to displacement damage due to radiation because the lattice constant of SiC is smaller than that of Si.

The reduction in p(T) by irradiation with 0.2 MeV electrons is less than that due to irradiation with 0.5 or 4.6 MeV electrons, although the larger amount of electrons was delivered to the sample in the case of the 0.2 MeV

Fig. 1. Temperature dependence of hole concentration for Al-doped ptype 4H-SiC before and after irradiation with electrons at three difference energies. (a) After Ref. [2].

electron irradiation. This suggests that the mechanism for the reduction in p(T) by irradiation depends on the irradiated electron energy.

In Fig. 1, the p(T) for the sample with irradiation of 0.2 MeV electrons is decreased at low temperatures, indicating that the N_{Al} was reduced with irradiation of 0.2 MeV electrons. On the other hand, the p(T) for this sample seems unchanged at high temperatures, suggesting that the sum of $N_{\rm Al}$ and $N_{\rm Defect}$ did not change by this irradiation. Therefore, with irradiation of 0.2 MeV electrons, the NAI was decreased, while the NDefect was increased.

The densities and energy levels of acceptors and defects can be determined by the FCCS. Using an experimental p(T), the FCCS signal is defined by [1,2]

$$H(T, E_{\rm ref}) \equiv \frac{p(T)^2}{(kT)^{5/2}} \exp\left(\frac{E_{\rm ref}}{kT}\right),\tag{1}$$

where k is the Boltzmann constant, T is the absolute temperature, and E_{ref} is the parameter that can shift the peak temperature of $H(T, E_{ref})$ within the measurement temperature range. The FCCS signal has a peak at the temperature corresponding to each acceptor level or defect level. From each peak, the density and energy level of the corresponding acceptor or defect can be determined accurately.

In the samples before and after irradiation, the values of an Al acceptor level (ΔE_{Al}), N_{Al} , a defect level (ΔE_{Defect}), N_{Defect} , and a compensating density (N_{comp}) were determined by the FCCS, and are listed in Table 1. In the

 10^{14} Before irradiation 10¹³ 0 0 After irradiation Δ : 0.2 MeV (1.0x10¹⁶ cm⁻²) : 0.5 MeV (5.0x10¹⁵ cm⁻²) 10^{12} : 4.6 MeV $(2.6 \times 10^{14} \text{ cm}^{-2})^{a}$ 8 9 2 3 5 6 7 1 4



Table 1
Results obtained by the FCCS for Al-doped p-type 4H–SiC epilayers before and after electron irradiation

Conditions	Before	After	Before	After	Before	After ^a
Energy (MeV) Fluence (cm ⁻²) ΔE_{A1} (meV) N_{A1} (cm ⁻³) ΔE_{Defect} (meV) N_{Defect} (cm ⁻³) N_{comp} (cm ⁻³)	203 5.2 × 10 ¹⁵ 357 3.5 × 10 ¹⁵ 4.7×10^{13}	$\begin{array}{c} 0.2 \\ 1.0 \times 10^{16} \\ 217 \\ 4.3 \times 10^{15} \\ 363 \\ 5.2 \times 10^{15} \\ 2.1 \times 10^{14} \end{array}$	204 4.8 × 10 ¹⁵ 319 2.3 × 10 ¹⁵ 1.9 × 10 ¹³	$0.5 \\ 5.0 \times 10^{15} \\ \\ \sim 2.6 \times 10^{14} \\ 356 \\ 1.4 \times 10^{15} \\$	203 6.2 × 10 ¹⁵ 365 4.2 × 10 ¹⁵ 3.4 × 10 ¹³	4.6 2.6 × 10^{14} 206 8.2 × 10^{14} 383 3.4 × 10^{15} 7.4 × 10^{14}

^aAfter Ref. [2].



Fig. 2. Relationship between N_{Al} and N_{Defect} . (a) After Ref. [1].

sample irradiated with $5.0 \times 10^{15} \text{ cm}^{-2}$ fluence of 0.5 MeV electrons, the values of ΔE_{Al} and N_{comp} could not be determined, because a reliable p(T) could not be measured at low temperatures. Each p(T) simulated with the values shown in Table 1 is in good agreement with the corresponding experimental p(T), indicating that the values determined by the FCCS are reliable.

Fig. 2 depicts the relationship between N_{Al} and N_{Defect} in each sample. The symbols of \triangle and \blacktriangle represent the relationships before and after irradiation with 0.2 MeV electrons, while the symbols of ∇ and \checkmark are the relationships before and after irradiation with 4.6 MeV electrons. The relationships in unirradiated epilayers with several doping densities are denoted by \circ , which were reported previously [1].

Since the empirical relationship in the unirradiated epilayers is obtained from Fig. 2 as

$$N_{\text{Defect}} = 0.6 \times N_{\text{Al}},\tag{2}$$

this defect is most likely related to Al. The irradiation with 0.2 MeV electrons resulted in a decrease in N_{Al} and an

increase in N_{Defect} , while the irradiation with 4.6 MeV electrons led to the decreases in both N_{Al} and N_{Defect} .

Although one of the possible origins of the unknown defect is B with which 4H–SiC is sometimes contaminated [4–6], the concentration of B in these epilayers, which was determined by secondary ion mass spectroscopy, was $<4 \times 10^{14}$ cm⁻³, indicating that B is not related to this defect. It may be closely linked with the D_1 line observed by PL [9] or with Al_{Si}–V_C observed by EPR [7].

The maximum energy (E_{max}) transferred from an electron to a nucleus is given by [10]

$$E_{\rm max} = \frac{2E_{\rm e}(E_{\rm e} + 2m_{\rm e}c^2)}{Mc^2},$$
(3)

where E_e is the incident electron energy, M is the atomic mass, m_e is the electron mass, and c is the velocity of light. In SiC, the threshold displacement energy (E_d) was reported as ~40 eV [11–13], which might depend to some extent on the conduction type, the growth techniques, and so on. This indicates that the atom at the substitutional site is displaced by the incident electron when $E_{\text{max}} \ge E_d$.

Fig. 3 shows the atomic-mass-unit dependence of the minimum electron energy (E_{min}) required for the displacement of the substitutional atom. Judging from the figure, one electron with $0.19 \sim 0.36$ MeV can displace only C_s.

With irradiation by 0.2 MeV electrons at 1.0×10^{16} cm⁻² fluence, the decrement of N_{Al} is nearly equal to the increment of N_{Defect} , as shown in Table 1. If the bond between Al_{Si} and its nearest neighbor C_s is broken due to the displacement of the C_s by this electron irradiation, the Al acceptor density is decreased and the density of the Al_{Si}-V_C complex is increased, which is consistent with our experimental finding. Therefore, the origin of the unknown defect is most likely Al_{Si}-V_C.

With irradiation by electrons at $\ge 0.5 \text{ MeV}$, the N_{Al} should decrease due to the displacement of both C_s and Al_{Si}. When the unknown defect is Al_{Si}-V_C, the N_{Defect} should decrease due to the displacement of Al_{Si}, while it should increase due to the displacement of the C_s closest to Al. Therefore, the N_{Al} is reduced significantly, whereas the N_{Defect} is decreased slightly, which is in good agreement with our experimental results.



Fig. 3. Atomic-mass-unit dependence of minimum electron energy required for displacement of substitutional atom in SiC.

4. Conclusion

We have investigated the reduction in p(T) for Al-doped p-type 4H–SiC epilayers with irradiation by electrons of several energies, and have determined the densities and energy levels of a shallow acceptor and a deep defect using FCCS. With irradiation by 0.2 MeV electrons, the shallow Al acceptor density was decreased, while the unknown deep defect density was increased. Since one 0.2 MeV electron could displace only C_s into an interstitial site, the Al acceptor density was decreased due to the displacement of the C_s closest to Al, which resulted in an increase in the density of Al_{Si}-V_C. Therefore, the deep defect is most likely Al_{Si}-V_C.

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