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Exploring the Ion Implantation Mechanism for Suppressing Stacking Fault Expansion in 4H-SiC: A Fundamental Approach

Takashi Yoda[1,a*], Masaki Sano[3,b], Jun Kojima[4,c], Shoichi Onda[4,d], Anton Myalitsin[1,e], Kuniyuki Kakushima[1,2,f], Takayuki Ohba[1,g], Atsushi Oshiyama[4,5,h] and Kenji Shiraishi[3,5,i]

[1]WOW Alliance, [2]School of Engineering, Institute of Science Tokyo, 4259 Nagatsuta, Midori-ku, Yokohama, 226-8503, Japan

[3]Graduate School of Engineering, [4]Institute of Materials and Systems for Sustainability, Nagoya University, Nagoya, Aichi 464-8603/8601, Japan

[5]Center for Innovative Integrated Electronic Systems, Tohoku University,Sendai, 980-8572, Japan

[a*]yoda.t.efe9@m.isct.co.jp, [b]sano.masaki.0328@outlook.jp, [c]kojima.jun.t2@f.mail.nagoya-u.ac.jp, [d]onda.shoichi.n9@f.mail.nagoya-u.ac.jp, [e]anton@anvos-analytics.com, [f]kakushima.k.aa@m.titech.ac.jp, [g]ohba.t.ac@m.titech.ac.jp, [h]atsushi.oshiyama.b5@tohoku.ac.jp, [i]kenji.shiraishi.c2@tohoku.ac.jp

Keywords: silicon carbide (SiC), power devices, basal plane dislocations (BPDs), Single Shockley-type stacking faults (1SSFs), proton implantation, density functional theory (DFT), photoluminescence (PL), cathodoluminescence (CL), carbon vacancies (V_c).

Abstract. Suppressing the expansion of Single Shockley-type stacking faults (1SSFs) is critical for the growing demand of high-performance power devices. However, the underlying suppression mechanism has not yet been fully elucidated. Through proton ion implantation studies, we have established a fundamental approach by modeling this phenomenon. Carbon vacancy (V_c) generated by high-energy proton implantation are found to play a significant role in suppressing the expansion of 1SSFs.

Introduction

Silicon carbide (SiC) power devices exhibit superior performance compared to conventional silicon-based counterparts, enabling operation at higher voltages and frequencies with enhanced power efficiency and reduced energy losses. However, during the epitaxial growth of SiC, basal plane dislocations (BPDs) propagate from the substrate into the epitaxial layer. Further complications arise from the fact that BPDs dissociate into pairs of partial dislocations (PDs) on the basal plane, accompanied by Single Shockley-type stacking faults (1SSFs), which expand when low-energy holes interact with the Si-core. The expansion of these 1SSFs leads to bipolar degradation [1]. Practical proposal to suppress the 1SSFs expansion have been actively developed and reported [2-11]. A standard solution is to design a recombination-enhancing buffer layer [12]. Proton implantation has also emerged as a promising technique for suppressing the formation of 1SSFs [13-16]. As alternative candidates, implantation techniques using helium and other ion species have been investigated [17-19]. More recently hydrogen plasma treatment, which causes less damage to the device, has also been reported [20]. At the early stage of proton implantation development, various mechanisms for suppressing 1SSFs expansion, including hydrogen-related effects, were actively discussed. Nevertheless, as research on helium and other ion implantations has advanced, the role of vacancies has increasingly come into focus. In this study, we evaluate the impact of proton implantation on the suppression of the expansion of 1SSFs. Furthermore, we investigate the underlying suppression mechanisms by analyzing the atomic and electronic structures surrounding the 1SSFs.

Experimental and Modeling

The epitaxial films used in this study consisted of a 10-µm-thick drift layer grown on an n-type 4H-SiC substrate. Two types of 4H-SiC epitaxial films were subjected to proton implantation at depths of 5 µm and 10 µm from the epitaxial surface, respectively. The proton implantation conditions were 0.6MeV for the 5-µm depth and 0.95MeV for the 10-µm depth, with an identical dose of 1×10^{15} cm^{-2}. Following proton implantation, the samples were irradiated with ultraviolet (UV) light to promote the expansion of 1SSFs. The UV irradiation was carried out using a 355nm Nd:YAG laser with an output power of 10W and a spot size of 3mm in diameter. Photoluminescence (PL) imaging through a 420-nm bandpass filter was employed to monitor the evolution of 1SSFs. Specimens for scanning transmission electron microscopy (STEM) were prepared using a focused ion beam (FIB) system (Helios 660, FEI). Cross-sectional STEM observations of 1SSF edges were performed with a JEM-ARM300F2 (JEOL) operated at an acceleration voltage of 300 kV. Cross-sectional cathodoluminescence (CL) measurements were conducted using a Schottky-emission scanning electron microscope (SEM, S-4300SE). The accelerating voltage was set to 10 kV with a beam current of ~2nA. CL spectra were collected at low temperature (28K) using a Si-CCD detector. For modeling basal plane dislocations (BPDs), 1SSFs, and vacancy structures, structural optimization and electronic state calculations were performed using the Vienna Ab initio Simulation Package (VASP), based on density functional theory (DFT) [21].

Results and Discussion

We first evaluated photoluminescence (PL) imaging of the 10-µm-thick drift layer of 4H-SiC following proton implantation at a depth of 5 µm from the epitaxial surface (Fig. 1). Figure 2 shows a bright-field STEM cross-sectional image corresponding to the region indicated by the red arrow in Fig. 1. The image clearly demonstrates that proton implantation effectively suppresses the expansion of 1SSFs. The expansion of 1SSFs was terminated by a partial dislocation (PD) located at 5.8 µm below the surface of the epitaxial layer, which is nearly identical to the targeted implantation depth of 5 µm. Subsequently, cross-sectional CL measurement s were performed for both the 5- µm and 10-µm proton-implanted epitaxial layers, as shown in Fig. 3 and 4. Three main features were identified in the spectra: near-band-edge emission (375-400nm), broad emission (430-700nm), and silicon vacancy (V_{Si})-related emission (852nm and around 950nm). Figure 5 shows the CL spectra near 380-nm peak wavelength, comparing the results for proton implantation depths of 5 µm and 10µm from the epitaxial film surface.

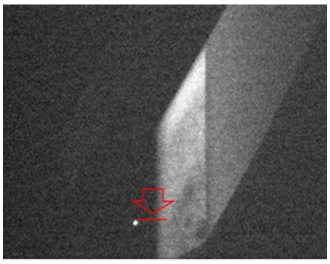

Fig. 1. PL-Imaging after proton implantation. Red arrow indicates STEM area.

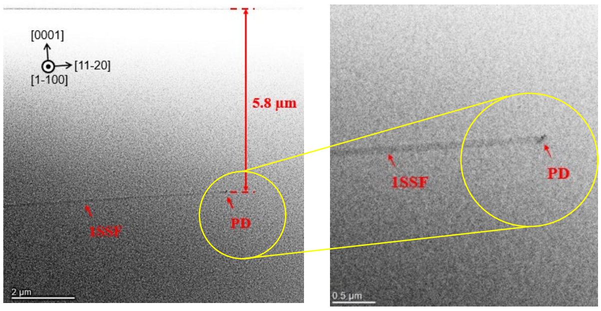

Fig. 2. BF-STEM cross sectional image of SSF expansion suppressed by proton irradiation.

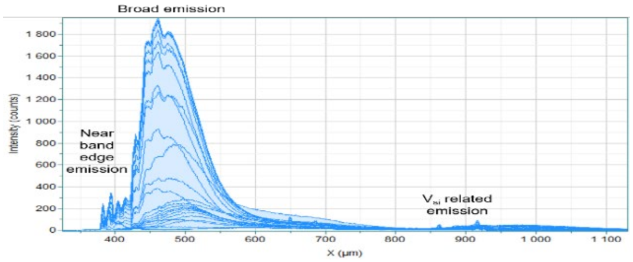

Fig. 3. CL spectra of 5µm depth proton irradiated sample.

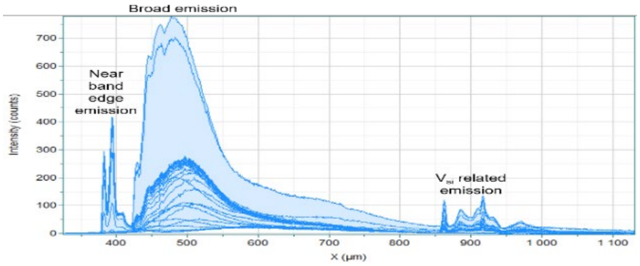

Fig. 4. CL spectra of 10µm depth proton irradiated sample.

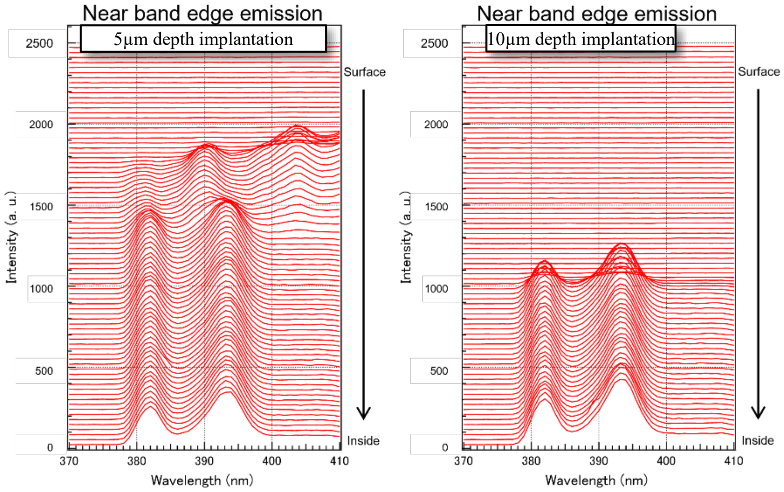

Fig. 5. Cross sectional CL spectra after proton implantation up to 5µm and 10µm from the epitaxial film surface.

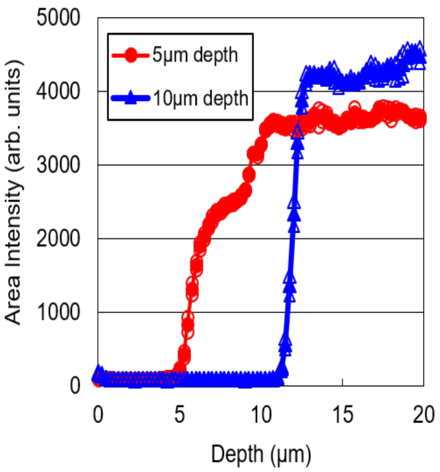

Fig. 6. CL area intensity depth profile between 5µm and 10µm depth proton implantation sample.

This peak is generally attributed to near-band-edge emission arising from transitions between the conduction band minimum (CBM) to the valence band maximum (VBM). The cumulative intensity distribution in the 375-400nm range is presented in Fig. 6. The data reveal that, up to the proton implantation depth, only weak emission signals are detected, suggesting the presence of non-emissive centers in the implanted region, most likely associated with vacancies. V_{Si}-related emission was also observed in Figs. 3 and 4. However, since the majority of intrinsic defects in 4H-SiC are carbon vacancies (V_C) due to their lower formation energy, the dominant defects are expected to be V_C rather than V_{Si}. It should be noted that CL measurements can sometimes enhance V_{Si}-related emission because of the deep and stable energy levels of V_{Si}. In this study, the specific vacancy type could not be conclusively identified. Vacancies generated by proton implantation are likely to include V_C, V_{Si}, and their complexes. However, considering the formation energies and experimental support from previous defect studies using deep level transient spectroscopy (DLTS) after proton implantation [16], in which a peak assigned to the $Z_{1/2}$ center (origination from V_C) was observed, V_C is the most favorable to form and thus represents the most plausible candidate. A Fundamental analysis of the dynamic behavior of defects during ion implantation has been reported in [22]. Building on these insights, we investigated the mechanism responsible for the suppression of 1SSF expansion induced by proton implantation. To this end, we incorporated carbon vacancies (V_c) near the expanded 1SSFs in our model and performed first-principles calculations. The employed model is illustrated in Fig. 7. The green ball in Fig. 7 denotes the nearest-neighbor Si atom, the brown dotted circle represents a carbon vacancy (V_c). According to our calculations, once a V_c is created, the nearest Si atoms form a pair to achieve stabilization. Analysis of the atomic distance after geometry optimization shows bond lengths of 2.71Å and 2.77Å, respectively. Compared with the typical Si-Si bond length in the Si-core (~2.4Å), the Si-Si pair distance is slightly larger.

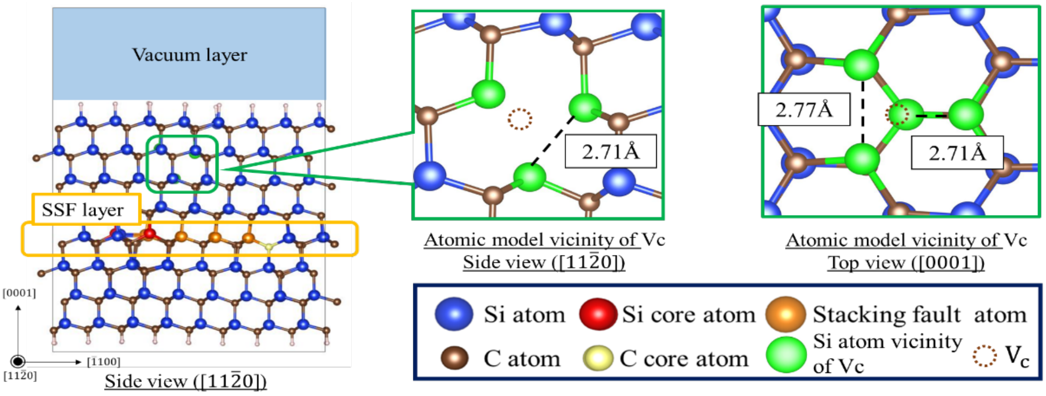

Fig. 7. Side view of the 4H-SiC model with SSF and V_C. Enlarged view of the model vicinity of the V_C are also depicted.

To clarify the influence of V_c on 1SSFs expansion, we carried out a Local density of states (LDOS) analysis. The results indicate that both the Si-Si bond beneath the V_c and the Si-Si bond in Si-core introduce electronic states within the bandgap. Notably, the Si-Si bond in the vicinity of the V_c is associated with deeper states within the bandgap. Based on these findings, we propose the following mechanism: when a V_c is located near a 1SSF, electrons associated with the Si-Si bond at V_c site may transfer to the Si-Si bond in the Si-core, which is responsible for hole trapping. Consequently, the occupied Si-core can no longer capture holes, thereby suppressing the expansion of 1SSFs (Fig. 8).

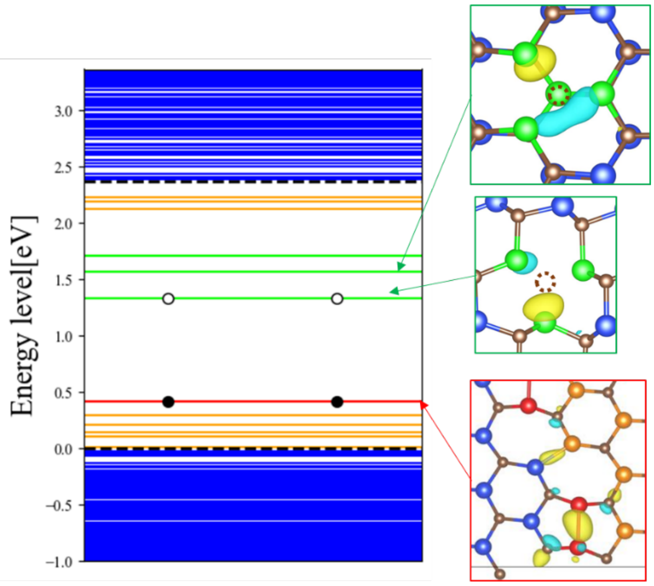

Fig. 8. The energy levels and wavefunctions of Si-Si bond in Vc (green energy level) and Si-Si bond in Si-core (red energy level), respectively.

Summary

In this study, we investigated the suppression mechanism of 1SSF expansion by evaluating the impact of proton implantation, with particular focus on vacancy-related effects, using cross-sectional CL spectra. In addition, we performed LDOS analysis to clarify the atomic and electronic structures around carbon vacancies. The results suggest that when carbon vacancies are formed in the vicinity of 1SSFs, suppressions of their expansion arises from the inhibition of hole capture at the Si-core by these vacancies. This study provides new insights into the mechanism of 1SSF suppression and may offer valuable guidance for future process improvement.

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