

高温 $N_2(+O_2)$ アニールにおける SiC の表面酸化反応によって変化する 4H-SiC/SiO₂ 構造へ N の取り込みと除去の速度論的バランスの理解

Understandings of the kinetic balance between N incorporation and removal affected by SiC surface oxidation for 4H-SiC/SiO₂ structure in high-temperature $N_2(+O_2)$ annealing

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[Motivation]

Improvement of the performance of 4H-SiC MOSFET was demonstrated by nitridation process, which was related to the density of surface N atoms incorporated during the interface nitridation process [1]. However, for the conventional nitridation process by NO post-oxidation annealing (POA), there is a plenty of room to improve the surface N density, which would be determined by the kinetic balance between the simultaneous reactions of N incorporation and N removal from the SiC surface during annealing. For designing a nitridation process to achieve a higher surface N density ($N(t)$, where t is the annealing duration), the control of such balance is critical. In case of NO annealing the N removal is attributable to the surface oxidation [2]. To simplify the model, we assume the reaction rate of N-incorporation (N_+) to be constant during POA, and the removal rate (N_-) to be proportional to the surface oxidation rate (R) and $N(t)$. Thus, the effective nitridation rate ($dN(t)/dt$) would be as follows:

$$\frac{dN(t)}{dt} = N_+ - N_- \Rightarrow N(t) = \frac{1}{c} \cdot \frac{N_+}{R} [1 - \exp(-cR \cdot t)], \text{ where } N_- = cR \cdot N(t) \quad (1)$$

where c is a constant. According to Eq. (1), $N(t)$ would saturate at a certain level that is determined by N_+/R , which could be experimentally determined. This study aims to provide systematic understandings of the kinetic balance between N incorporation and N removal based on Eq. (1) for 4H-SiC(0001)/SiO₂ structures. For this purpose, the high-temperature N_2 -POA was used in this study to control N_+ and N_- independently by tuning R with intentional O_2 introduction instead of annealing in NO that decomposes to produce O_2 with poor controllability.

[Experimental]

4°-off 4H-SiC(0001) with epitaxial layer ($\sim 1 \times 10^{16} \text{ cm}^{-3}$ n-type doped) were used as substrates. After oxidizing in dry O_2 to grow around 6nm-thick SiO₂ layer, POA was done at 1370°C from 1 to 45min in N_2 ambient, with a series of small amount of O_2 whose partial pressure was denoted as P . The SiO₂ regrowth thickness (ΔT_{OX}) during N_2 -POA was determined by measuring X-ray reflectivity before and after POA. After removing the SiO₂ layer completely with HF, the relative ratio of N (N/Si) was estimated with the peak area ratios of N1s to Si2p by XPS.

[Results and discussions]

Fig. 1 shows the t dependence of N/Si as well as ΔT_{OX} (inset) for a series of P . Saturation of N/Si is found for large t . The saturated surface N concentration (N_{sat}) was determined by fitting the $N/Si - t$ relationship with the exponential function shown by Eq. (1). The initial nitridation rate $N_r^{ini} (= [N/Si(t)]/t)$ in the initial stage of POA was defined to approximately estimate N_+ , while the oxide growth rate \bar{R} was determined from the slope of $\Delta T_{OX} - t$ relationship. Fig. 2 summarized the P dependence of N_r^{ini} and N_r^{ini}/\bar{R} . Note that N_r^{ini} increases with P , which means a slight addition of O_2 enhances N_+ . This is explainable considering that the incorporation reaction would be triggered by surface oxidation [3]. On the other hand, N_r^{ini}/\bar{R} decreases monotonously with P , indicating that the enhancement of N_- by oxidation is more significant than that of N_+ . Fig. 3 shows the relationship between N_{sat} and N_r^{ini}/\bar{R} . A linear relationship was observed, which clearly shows that N_r^{ini}/\bar{R} is a good indicator for saturated surface N density rather than P . P would affect N_r^{ini}/\bar{R} since N_+ and N_- show quantitatively different relationships with P , and therefore have an impact on N_{sat} . Besides, a higher N_{sat} was found for $P = 0$ cases (data not shown), which will be explainable by taking the active oxidation rate as N_- instead of \bar{R} in the passive oxidation cases.

[Conclusions]

While a slight amount of O_2 inclusion in N_2 -POA ambient was found to enhance N_+ , the parameter N_+/R was verified to be a good indicator of the incorporation-removal balance which determines N_{sat} .

[Acknowledgement] This work was partially supported by JSPS KAKENHI.

References [1] J. Rozen et al. J. Appl. Phys. **105**, 124506 (2009). [2] K. McDonald et al., J. Appl. Phys. **93**, 2257 (2003). [3] T. Yang et al. Extended Abstract of the 8th ADPS Conference (2021) IIA-9.

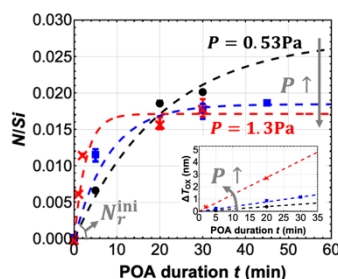


Fig.1 t dependence of N/Si and ΔT_{OX} for different P .

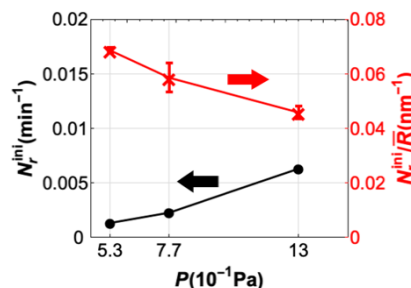


Fig.2 P dependence of N_r^{ini} and N_r^{ini}/\bar{R} .

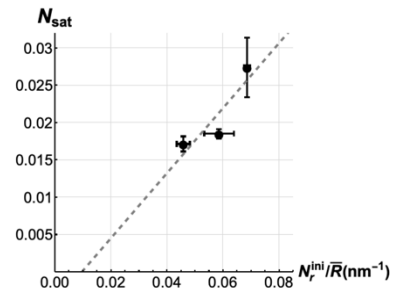


Fig.3 Relationship between N_{sat} and N_r^{ini}/\bar{R} .