Thermal-oxidation-induced Lattice Distortion at 4H-SiC (0001) Surface and Its Recovery by Ar Annealing

熱酸化された 4H-SiC（0001）表面に局所的に生じる格子歪みと Ar アニールによる回復

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[Background] Recently, oxidation-induced macroscopic distortion due to the bending of SiC wafer caused by the formation of thermally-oxidized SiO_2/4H-SiC interface was studied [1]. In addition to such macroscopic one, however, distortion locally in the vicinity of the interface is also expected, taking account that thermal oxidation process of SiC is expected to generate SiO_2/4H-SiC interface with an interstitial-incorporated 4H-SiC layer in a proposed oxidation mechanism [2]. It has also been theoretically predicted [3] that the formation of interface states may partly originate from change in electrical structure of 4H-SiC associated with strains in 4H-SiC. In this report, we investigated the thermal-oxidation-induced lattice distortion at surface of 4H-SiC (0001) and its recovery by post-oxidation Ar annealing, characterized by in-plane X-ray diffractometry (XRD).

[Experimental] N-type (4° off-axis) 4H-SiC (0001) Si-face wafers covered with 5 µm epitaxial layers were used as substrates. Dry oxidation processes at 1300 °C for various time were performed followed by post-oxidation annealing in O_2 at 800 °C for 30 min. Post-oxidation Ar annealing processes were then performed at 1150 and 1300 °C for various time after oxide removal in diluted HF. NO annealing (in 33% NO diluted by N_2) was also performed at 1150 °C for 2 hr for comparison. All samples were characterized by using in-plane XRD to determine the interspacing of lattice planes perpendicular to the wafer surfaces. The shallow incident angles from 0.23 to 1.25 degree were employed to limit the X-ray penetration depth.

[Results and discussion] SiO_2 layers with thicknesses of 12, 29, and 44 nm were thermally grown by performing dry oxidation for different time. **Fig. 1(a)** shows the relationships between $d_{(1\bar{1}00)}$ interplanar spacing and X-ray penetration depth for the oxidized 4H-SiC with different SiO_2 thickness. $d_{(1\bar{1}00)}$ of the sample was higher in shallow area, and lower in deeper area. Furthermore, a larger $d_{(1\bar{1}00)}$ value was observed from the samples with thicker oxide layers, which indicated that a longer oxidation time induced larger lattice distortion [4], due to the larger amounts of generated defects. Next, post-oxidation Ar annealing was performed to clarify the possibility of lattice distortion recovery. **Fig. 1 (b)** shows the effects of Ar annealing time on the lattice distortion recovery. It indicates that Ar annealing could partially reduce the lattice distortion, while the longer annealing time resulted in the larger recovery. We speculated this Ar annealing process should cause the migration and removal of accumulated defects that cause the lattice distortion at the surface of 4H-SiC. Furthermore, we examined the lattice distortion at the surface of NO-annealed sample and found that the impact of NO annealing on the lattice distortion recovery was almost the same as Ar annealing, as shown in **Fig.2**. In conclusion, the thermal-oxidation-induced lattice distortion at surface of 4H-SiC (0001) was clearly observed by in-plane XRD measurements. It could be partially recovered by post-oxidation Ar annealing, while the recovery was larger for longer annealing time. Our results revealed that oxidation and annealing processes should have a significant impact on the quality of the 4H-SiC surface.

Acknowledgments. This work was partly supported by CSTI, Cross-ministerial Strategic Innovation Promotion Program, "Next-generation power electronics" (funding agency: NEDO), and by JSPS KAKENHI.

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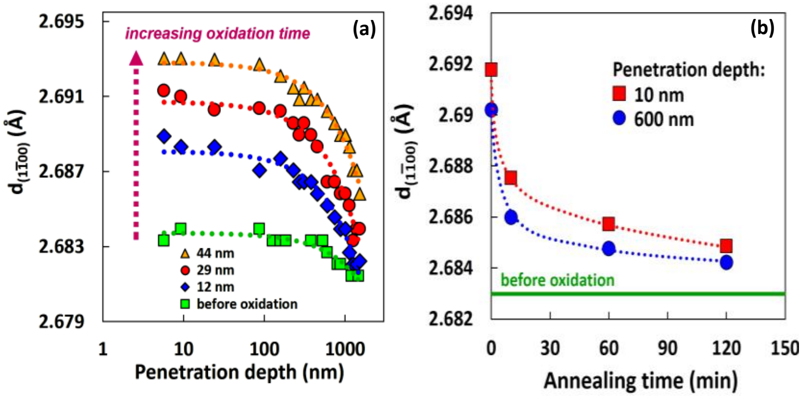

Fig. 1. (a) Penetration depth dependence of $d_{(1\bar{1}00)}$ of SiO_2/4H-SiC with different SiO_2 thicknesses, and **(b)** the effect of Ar annealing time on the lattice distortion recovery.

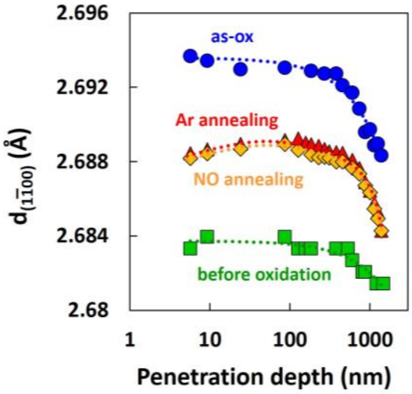

Fig. 2 Comparison between the impact of Ar and NO annealing on the lattice distortion recovery.