熱酸化による 4H-SiC 表面での格子歪みの起源となる残留副生成物の物理分析

Physical Analysis of Remained Oxidation Byproducts as the Origins of Lattice Distortion at 4H-SiC Surface

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[Introduction] We have reported an oxidation-induced significant lattice distortion of SiC, locally in the vicinity of the SiO_2/SiC interface and its relaxation by Ar annealing [1]. From the kinetic studies it was also suggested that the formation and decomposition of oxidation-induced byproducts in the surface region of SiC are one of the possible mechanisms [2], even though the existence of such remaining byproducts have not yet been physically clarified. In this work, we investigate the chemical bonds in thermally-oxidized 4H-SiC surface region by Fourier-transform infrared spectroscopy with attenuated total reflection mode (FTIR-ATR) to physically clarify the existence of remaining byproducts of thermal oxidation in the surface region.

[Experimental] Wafers of 4° off-axis 4H-SiC (0001) with 5 μm-thick n-type doped (~1×10^{16} cm^{-3}) epitaxial layers were used as substrates. After cleaning the wafer, dry oxidation in 1 atm oxygen (O_2) gas at 1300°C was performed, followed by annealing in O_2 at 800°C for 30 min. Argon (Ar) annealing was then performed at 1300°C after total oxide removal in diluted hydrogen fluoride (HF) solution. All samples were characterized by in-plane X-ray diffractometry to determine the interplanar spacing of lattice planes perpendicular to the wafer surfaces. FTIR analysis with ATR mode using germanium crystal with 45° incidence angle was then performed to determine the possible structure of remained byproducts at the top 1 μm-deep 4H-SiC surface.

[Results and discussions] FTIR-ATR spectra of as-oxidized 4H-SiC and after 120 min Ar annealing are shown in **Fig. 1**. The result of the as-received wafer is also shown for comparison. FTIR spectra of the as-oxidized sample shows, in common, the absorption at the wavenumber of around 838, 1295 and 1540 cm^{-1}, whereas the 4H-SiC wafer before oxidation does not show the peaks in those wavenumbers. Those peaks are attributable to Si-O bending, C-O stretching, and conjugated C=O asymmetric stretching vibration [3,4], respectively. The absorption of these O-related structure can then be reduced significantly by Ar annealing. The relationship between surface lattice distortion (D, increase ratio of $d_{(1\bar{1}00)}$ of 4H-SiC) and the concentration of O-related structure in 4H-SiC surface is then studied. **Fig. 2** summarizes the lattice distortion of the samples with different Ar annealing time determined by in-plane XRD with ~10 nm X-ray penetration depth condition, as a function of intensity of infrared absorption at the wavenumbers of around 838, 1295 and 1540 cm^{-1}. The absorption intensity at each wavenumber of all samples was normalized by the peak of the longitudinal optical phonon mode of SiC which observed at the wavenumber of around 970 cm^{-1} [5]. It shows that the change of lattice distortion is observed to be roughly proportional to the change of concentration of O-related structure, which represented by the IR absorbance at those specific wavenumbers. Our results revealed that the existence of oxidation byproducts as a form of O-related structure could be physically confirmed to be remained at 4H-SiC surface and considered as the origin of surface lattice distortion.

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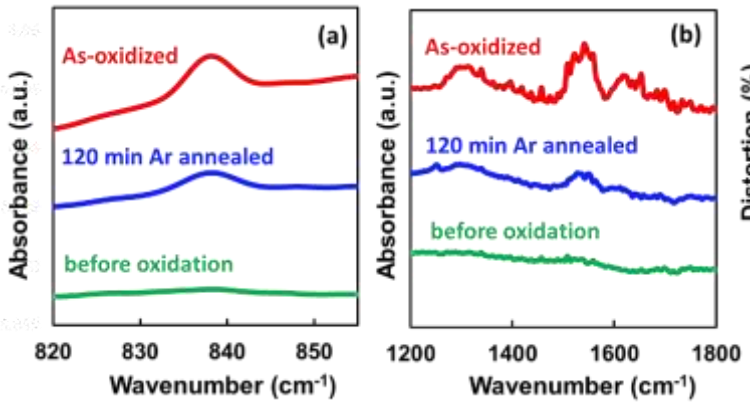

Fig. 1 FTIR-ATR spectra of as-oxidized 4H-SiC and after Ar annealing at 1300°C for 120 min in the range of wavenumber of **(a)** 820-860 cm^{-1} and **(b)** 1200-1800 cm^{-1}. The spectra of before oxidation are also shown for comparisons.

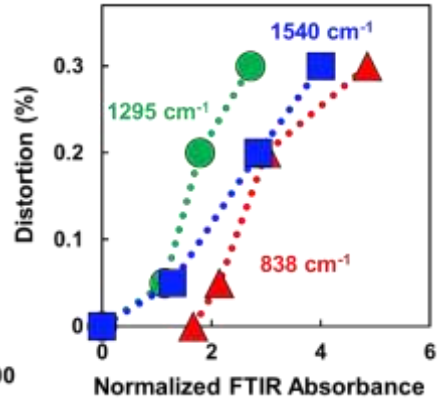

Fig. 2 Relationship between the lattice distortion determined by in-plane XRD with penetration depth of ~10 nm, and the normalized infrared absorbance at the wavenumbers of 838, 1295 and 1540 cm^{-1}.