

Chemical structure of the SiO₂/Si(001) interface formed at high temperatures

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An understanding of thermal silicon oxidation is essential for further advancements in semiconductor science and technology. Of particular importance is that we clarify the mechanism of the morphological evolution between the growing thermal silicon oxide layers and Si(001) substrate during oxidation so that we can obtain an abrupt interface on an atomic scale. This is because the morphological features, including roughness and atomic steps at the SiO₂/Si(001) interface seriously degrade the dielectronic properties of silicon devices, such as metal-oxide-semiconductor field emission transistors (MOSFETs).

Thermal silicon oxidation, in general, can be categorized according to oxidation temperature as low-temperature (400 – 1100°C) or high-temperature [1100 – 1414°C (melting point of Si)] oxidation. Thermal oxidation at low temperature is widely used to obtain insulating silicon oxide layers in conventional Si devices, and the chemical structure of the SiO₂/Si(001) interface has been extensively studied so far. Thermal silicon oxidation at high temperature, on the other hand, is becoming important for advanced silicon devices based on silicon-on-insulator (SOI) structures.[1] However, little attention has been paid to the chemical structure of the high-temperature thermally grown silicon oxide layers on Si(001) and its interface.[2] The chemical information at the interface is essential for understanding the origin of the interface roughness.

Here, we report a photoemission study of the thermally grown SiO₂ on Si(001) at high-temperature.

We used B-doped Si(001) wafers with miscut angle of

1°. The wafers were thermally oxidized in conventional electronic furnace. The wafers were subjected to various annealing conditions in an Ar atmosphere containing a small constant fraction of O₂ gas (0.2%). Annealing temperatures and times were 1200, 1250, and 1325°C, and 2.5, 4, and 2.5 h. The silicon oxide layers were etched back in dilute HF solution (1%) followed by DI water rinse. The etchback oxide thickness was less than 5 nm and the etchback treatment did not destroy the buried SiO₂/Si interface.

A typical spectrum recorded at 240 eV photon energy from a 1250°C sample shows that different suboxide peaks are clearly observed in the raw data. The peaks can be assigned to the suboxide states (Si⁺¹, Si⁺², Si⁺³, Si⁺⁴). The intensities of the Si⁺¹, Si⁺², Si⁺³ peaks become strong with increasing incident beam energies, indicating that the suboxide states are localized at the interface. The observed intensity distribution is quite different with that of the SiO₂/Si(001) interface formed at low temperatures. This discrepancy means that the high-temperature thermal silicon oxidation produces the original chemical states at the interface.

References

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