1Ia03Y **Influence of hafnium chemical state difference on initial silicon oxidation at interface between hafnium deposition and Si(100) substrate**

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Hafnium dioxide (HfO_2) has promising potential for alternative material of silicon dioxide (SiO_2) which is employed as typical gate oxide film in metal-oxide-semiconductor field effect transistor (MOSFET) because of a high permittivity ($k \approx 21$), a large bandgap (~5.7 eV), and a thermal stability[1, 2)]. The application of ideal HfO_2 film allows us to reduce effective thickness of gate oxide film continuously without serious leakage current which happens through ultrathin SiO_2 gate film. Therefore, to understand the oxidation dynamics at surface and interface of ultrathin hafnium (Hf) film composed on Si(100)-2×1 [Hf/Si(100)] is one of the most significant issues for sustainable development of Si semiconductor devices. In this study, we investigated Hf and silicon (Si) oxidation processes depending on different Hf chemical states by means of the Si $2p_{1/2,\ 3/2}$, Hf $4f_{5/2,\ 7/2}$, and O 1*s* core-level photoelectron spectroscopy combined with synchrotron radiation soft X-ray at BL23SU of SPring-8.

As our result, Hf and Si in Hf/Si(100) are immediately oxidized up to be HfO_2 (Hf^{4+}) and SiO_2 (Si^{4+}) by exposure to O_2 molecules because metallic Hf component which generates just after Hf deposition works like oxidation enhanced catalysis[3)]. On the other hand, the metallic Hf component could be turned into island Hf disilicide component [*i*-$HfSi_2$/Si(100)] after annealing around 1073 K. After exposure the *i*-$HfSi_2$/Si(100) to O_2 molecules, the *i*-$HfSi_2$ hardly reacts with O_2 molecules because it doesn't act as catalysis. Therefore, the oxidation of Si(100) substrate was suppressed drastically.

Our study indicates that the Hf chemical states have a major influence on Si oxidation dynamics.

References

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