Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Intrinsic Effect of a Nitrogen Atom on Hf-based High-k Gate Dielectrics -A First Principles Study NAOTO UMEZAWA, NIMS, Tsukuba, KENJI SHIRAISHI, Univ. Tsukuba, TAKAHISA OHNO, NIMS, Tsukuba, HEIJI WATANABE, Osaka Univ., Osaka, TOYOHIRO CHIKYOW, NIMS, Tsukuba, KAZUYOSHI TORII, Selete, Tsukuba, KIKUO YAMABE, Univ. Tsukuba, KEISAKU YAMADA, Waseda Univ., Tokyo, HIROSHI KITAJIMA, TSUNETOSHI ARIKADO, Selete, Tsukuba — We theoretically investigate the nitrogen incorporation effect in hafnia (HfO_2) from the first- principles calculations within GGA framework, especially focusing on the interaction between N atoms and O vacancies (Vo)s. Vo is known to be problematic for Hf-based high-k gate dielectrics because it causes unfavorable charge trap. Moreover, some experimental results suggest that Vo related gap statesassist the electron leakage current, which deteriorates the electrical properties of Hf-based MOSFETs. Our results clearly show that N atoms selectively occupy nearby O sites of Vo and that Vo levels are completely eliminated by the N incorporation. These results clearly show that N atoms have intrinsic effects to decrease Vo related gap states, leading to the reduction in both the number of charge trap sites and the leakage current through HfO_2.

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Date submitted: 05 Dec 2004 Electronic form version 1.4