Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

First-principles study of Fermi-level pinning at Al/SiON/SiC(0001) interfaces YASUNOBU ANDO, YOSHIHIRO GOHDA, SHINJI TSUNEYUKI, Depertment of Physics, The University of Tokyo — Schottky barrier generally emerges at metal-semiconductor interfaces and its height could ideally be estimated from the difference between the work function of the metal and the electron affinity of the semiconductor, which is called Schottky limit. However, for many semiconductors such as silicon, this condition is not satisfied due to the presence of interface states, which is referred as Fermi-level pinning. Recently, spectroscopic measurements and first-principles calculations showed that silicon oxynitride (SiON) formed on a 6H-SiC (0001) surface has a band gap as large as crystalline SiO_2. [T. Shirasawa, Y. Ando, S. Tsuneyuki, and H. Tochihara, et.al., PRB 79, 241301(R) (2009).] Since the Schottky barrier height depends on the kind of the metal at metal-SiO_2 interfaces, we expect that SiON on SiC also does not exhibit Fermi-level pinning. In this study, we have investigated electrostatic properties of Al/SiON/SiC and Al/Si interfaces based on density functional theory. Effects of the applied electric field have also been studied using the effective screening medium (ESM) method [M. Otani and O. Sugino, PRB 73 115407 (2006).] We have found that distribution of the internal electric field induced by the applied field is qualitatively different between them. Further, Al/SiON/SiC has less interface states than Al/Si, which is indicative that Al/SiON/SiC is in the Schottky limit.

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Date submitted: 20 Nov 2009 Electronic form version 1.4