Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Point Defects in Al_2O_3 and their impact on novel CMOS performance JUSTIN WEBER, Department of Physics, UC Santa Barbara, ANDERSON JANOTTI, CHRIS VAN DE WALLE, Materials Department, UC Santa Barbara — The desire for III-V CMOS devices has stimulated interest in novel dielectrics, which form high-quality interfaces III-V semiconductors. Recent significant progress has been reported using Al_2O_3. However, there is concern about defects that could degrade device quality. Therefore, we have performed a first-principles study of point defects in Al_2O_3. We analyze native point defects such as vacancies, self-interstitials, antisites, and dangling bonds, as well as hydrogen-related defects. Our first-principles calculations utilize state-of-the-art hybrid-functional methods within the HSE formalism. We also use calculated band offsets to make predictions about the location of defect levels with respect to the band edges of relevant III-V semiconductors. We find that the oxygen vacancy defect introduces defect levels near the conduction-band edge of relevant channel materials. Also, we find that vacancies can be responsible for accumulation of fixed charge in the crystal. Finally, hydrogen is considered as a passivation agent for defect states and fixed charge introduced by vacancy-related defects. Work supported by the Semiconductor Research Corporation and by NSF.

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Date submitted: 19 Nov 2009 Electronic form version 1.4