Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Valence band offsets and interface structure of HfxSi1-xO2 films on Si(111) from photoemission spectroscopy[1] JOHN ROWE, University of North Carolina, LES FLEMING, GERRY LUCOVSKY, North Carolina State University, MARC ULRICH, Army Research Office — We have used synchrotron radiation to perform high resolution soft x-ray photoemission spectroscopy measurements on Si(111)/$Hf_xSi_{1-x}O_2$ films. Our samples included both thick ($\sim$ 75 Å) and thin ($\sim$ 10 Å) silicate films. All samples were grown by remote plasma enhanced chemical vapor deposition (RPECVD) at a temperature of 300 °C using hafnium tert-butoxide and silane in a helium carrier gas. Si $2p$ and Hf $4f$ core levels were studied along with valence band spectra using photon energies of 64 and 150 eV. Measurements of the valence band edge were also unexpectedly high for the thick silicates, which may be attributable to bound charge in the form of defects in the films. The band offset parameter was estimated for the thin film compositions based on the Si $2p_{3/2}$ substrate peak position and its known binding energy with respect to the Si valence band edge (98.75 eV). Offsets for the thin film silicates ranged from 3.31 – 3.9 eV, with an average value of 3.42 $\pm$ 0.03 for x $>$ 0.2. Core-level binding energies exhibit a nonlinear dependence with alloy composition in the thick silicate films, while the thin films show a linear dependence. A decrease in binding energy for both the Si $2p_{3/2}$ [Si^{4+}] and Hf $4f_{7/2}$ was observed as the composition changed from SiO_2 to HfO_2.

[1]measurements erformed at NSLS - Brookhaven National Laboratory

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Date submitted: 05 Dec 2004 Electronic form version 1.4