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Conduction Band Tail States at GeO₂/Ge Interface Probed by Internal Photoemission Spectroscopy

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[Introduction] Band line-up determination at the semiconductor/insulator interface is essential to model the carrier transport properties of CMOS devices. Previously, we have reported a systematic band alignment determination at thermally-grown GeO₂/Ge interface by internal photoemission spectroscopy (IPE) and x-ray photoelectron spectroscopy (XPS).^[1] In this study, we further report an observation that although conduction band offset (CBO) is not sensitive to the GeO₂ thermal oxidation pressure, while the conduction band tail states can be effectively wiped off by increased oxidation pressure probed by IPE.

[Experimental] Thermally-grown GeO₂ under high pressure (70 atm, HPO) and atmospheric pressure (1 atm, APO) were prepared using the HF-last cleaned p-type Ge (100) substrate at 530°C for 60min (25nm thickness), then followed by low temperature O_2 annealing (LOA) at 380 °C for another 60min in O_2 atmosphere to repair GeO₂/Ge interface. MOS capacitors were then defined by thermal evaporation of semitransparent 15-nm-thick metal gate electrodes for IPE measurements. IPE spectral curves were recorded with 0.02 eV energy resolution in the photon energy ranging from 1.3 eV to 5 eV with the quantum yield (Y) defined as the photocurrent normalized by the incident photon flux.

[Results and Discussion] Fig. 1 displays a series of $Y^{1/3}$ -hv plots with the variance of substrate type for APO and HPO samples when the GeO₂/Ge MOS capacitors were measured under the same average strength of electric field (0.72 MV/cm) in the oxide insulator. The threshold extracted at zero quantum yield represents the energy barrier height between the valence band maximum of Ge and the conduction band minimum of GeO₂, thus the CBO at GeO₂/Ge interface can be determined by subtracting the reported Ge band gap (0.67 eV) from the as-determined threshold above. No significant difference of threshold determined from the spectral interval (2.4eV-2.8eV) was observed, indicating insignificant sensitivity of CBO on the oxide growth pressure, although HPO show significant improvement of GeO₂ bulk quality previously.^[2] Interestingly, the band tail states probed in the sub-threshold regime show a significant shift to higher photon energy for HPO compared to APO, which was more clearly observed to be ~ 0.2 eV from the $\log Y^{1/3}$ - plots (Fig. 2). The current observation suggests that HPO can effectively wipe off the band tail states emerged for APO GeO_2 at the GeO_2/Ge interface, and Fig. 3 shows the schematic band structure of thermally grown GeO₂ probed by IPE in this study.

[Conclusion] The conduction band tail states at GeO_2/Ge interface can be effectively wiped off by increased thermal oxidation pressure, although CBO is not sensitive to the oxidation pressure.





of substrate type for APO and HPO samples.

the sub-threshold regime.

