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XPS による GeO_2/Ge 界面の価電子帯バンドオフセットの決定

The Valence Band Offset at GeO_2/Ge Interface Determined by Charge-corrected XPS

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Introduction The band line-up determination at GeO_2/Ge interface is essential for modeling the transport properties of GeO_2 passivated Ge-based CMOS stacks, while the reported valence band offset (VBO) by XPS scattered ~ 1.0 eV. Previously, we have reported that the charging artifact is crucial to determine the VBO for XPS measurement, and the VBO has been calibrated to be 3.6 ±0.2 eV by referring to the shortest irradiation time.[1] Here, we give a more precise calibration of the VBO value by using the thinnest GeO_2 as the energy reference with the shortest irradiation time.

Experimental Thermally-grown GeO_2 with different thickness were produced using the HF-last cleaned p-type Ge (100) substrate at a temperature ranging from 450 to 530℃ in 1atm oxygen. The thickness and VBO were analyzed by XPS.

Results and Discussion In our previous study, Ge^{4+} and O1*s* signals have been revealed to increase sharply then reached a saturation value with the prelonged irradiation time. These signals were further observed to progressively shift toward higher binding energy with the increase of the GeO_2 thickness ranging from 2.58nm to 5.76nm even under the single sweep, which further indicates the differential charging effect of upper GeO_2 and Ge substrate during the XPS measurement (**Fig. 1**). To further calibrate the charging artifact on the VBO determination, the valence band edge energies were shifted by the value given by the difference between the respective O 1*s* or Ge^{4+} peak position and the thinnest GeO_2 thickness due to its minimal charging. Thus the VBO at GeO_2/Ge interface was finally found to be 3.45±0.2 eV for all oxides regardless of thickness, as shown in **Fig. 2**. Such result is consistent with our reported IPE result and **Fig. 2** inset shows the reconstructed band diagram.

Conclusion The constant VBO of 3.45±0.2 eV was obtained at GeO_2/Ge interface regardless of thickness.

Reference [1] W.F. Zhang, T. Nishimura, K. Nagashio, K. Kita, and A. Toriumi, SSDM, 731-732 (2012)

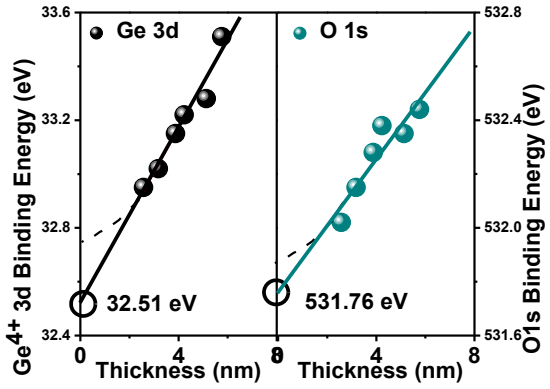

Fig. 1 Ge 3d and O 1*s* peak position of the GeO_2/Ge stacks with a single sweep as a function of different GeO_2 thickness.

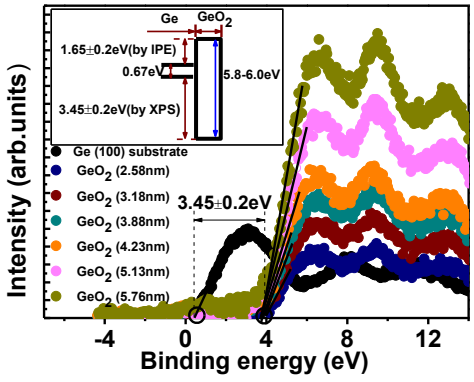

Fig. 2 Deconvoluted valence band spectrum of GeO_2 with different thickness, and the inset shows the reconstructed band diagram.