

Supporting Information

Influence of co-reactants on surface passivation by nanoscale hafnium oxide layers grown by atomic layer deposition on silicon

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Contents

S1. Thickness measurements and optical properties of O ₂ -HfO _x , O ₃ -HfO _x and H ₂ O-HfO _x	2
S2. Evolution of Hf 4 <i>f</i> peak contributions with milling duration	3
References	4

S1. Thickness measurements and optical properties of O₂-HfO_x, O₃-HfO_x and H₂O-HfO_x

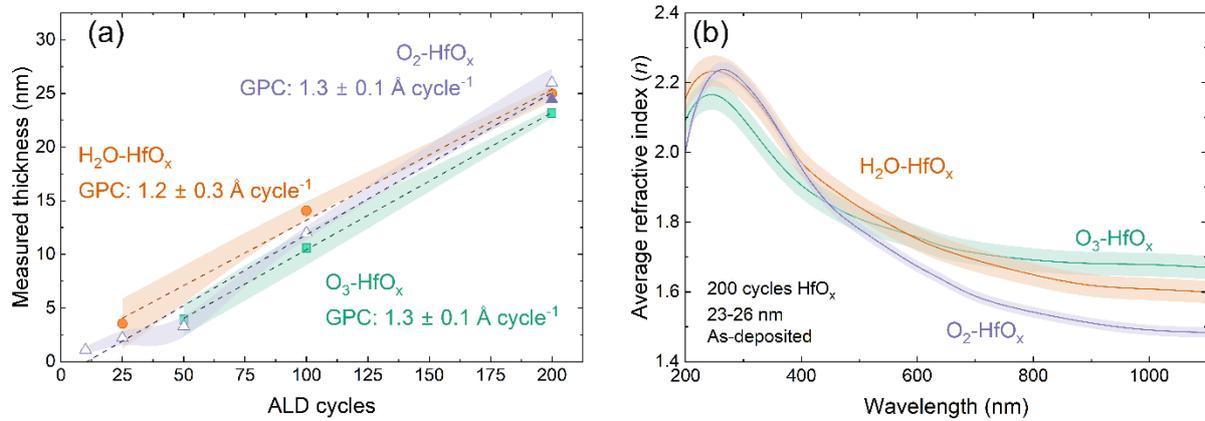


Figure 1: (a) Film thickness determined via spectral reflectivity as a function of number of ALD cycles for HfO_x on Si grown with different co-reactants (O₂ plasma (purple triangles), O₃ (green squares) and H₂O (orange circles) with a TDMAH precursor. Open shapes have been determined and reported previously.¹⁻³ Connections between points serve as a guide to the eye. Reported thicknesses are the average of five measurements, and the shaded region corresponds to the experienced uncertainty/variation between samples. The gradient of a line of best fit is taken as the growth per cycle (GPC). (b) Refractive indices for as-deposited O₂-HfO_x (purple), O₃-HfO_x (green) and H₂O-HfO_x (orange) as a function of wavelength. Plotted refractive indices are the average of five measurements, and the shaded region corresponds to the experienced variation across a sample.

S2. Evolution of Hf 4f peak contributions with milling duration

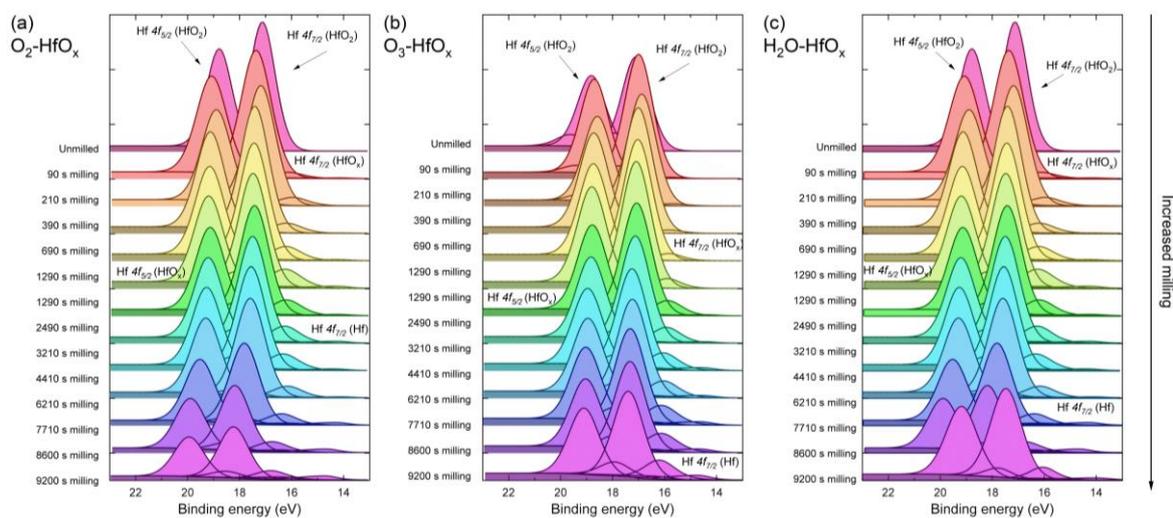


Figure S2: Deconvoluted Hf 4f XPS signal, showing Hf 4f_{5/2} and Hf 4f_{7/2} contributions for (a) O₂-HfO_x, (b) O₃-HfO_x, and (c) H₂O-HfO_x for different milling durations. Each film was ~25 nm thick and grown through 200 ALD cycles. Following 9200 s Ar⁺ milling, < 5 nm of HfO_x remains.

References

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<https://doi.org/10.1109/JPHOTOV.2022.3227624>.