



AN 415

Thin Film Hafnium Oxide (HfO₂) Thickness, Composition, and Uniformity Measurements by XPS

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Discussion

Fabrication of high- κ dielectrics such as HfO₂, used in semiconductor devices as a gate dielectric or capacitor dielectric, will require precise control of the film thickness, composition and stoichiometry, as well as film uniformity across a wafer and wafer-to-wafer. Failure to monitor and control any one of these factors will adversely affect the device performance and yield of the process. A HfO₂ *High Precision XPS Measurement* has been developed to characterize thin HfO₂ films on Si. Prior to this measurement, no one single technique could provide all of this information about the dielectric film in a rapid, precise, and cost-effective manner.

Semiconductor manufacturers, semiconductor process development groups, and deposition tool manufacturers need to control multiple properties of these ultra-thin dielectric films as early in the deposition process as possible to reduce costs and improve yields. Process development in particular requires feedback quickly and precisely in order to meet customer requirements for process tool design and performance. The deposition tool suppliers, be it MOCVD, PVD, or especially ALD, need to demonstrate the performance of their tools in depositing highly uniform ultra-thin films with constant composition and stoichiometry, and reliable thickness control.

As noted above, high- κ dielectric performance requires not only precise film thickness control, but because the dielectric constant is so high it is also very sensitive to compositional or stoichiometric changes. In the case of deposition of HfO₂ films on Si, the HfO₂ film has an interfacial layer of either SiO₂ or Hf_xSi_(1-x)O₂ (see Figure 1) that can substantially change the overall dielectric property of the film. (This is typically referred to as Equivalent Oxide Thickness, EOT, of an ideal equivalent SiO₂ film.) Therefore it is not only imperative to know the HfO₂ film thickness but also the interfacial silicate or SiO₂ film thickness. Thickness of both layers are possible with the HfO₂ *High Precision XPS Measurement*. For purposes of illustration, Table 1 shows the interfacial layer thickness and the HfO₂ thickness as determined by this measurement. The values in the first row of the table are the averages obtained from over 30 measurements across a Si wafer containing a thin HfO₂ layer.

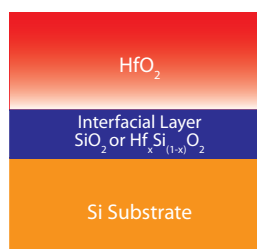
Table 1. Layer Thicknesses and Stoichiometry of a thin HfO₂ film on Si

	Interfacial Layer Thickness (Å)	HfO ₂ Thickness (Å)	Corrected O:Hf ratio
Avg.	12.14aa	39.95	2.50
Std. Dev. (1σ)	0.22	0.33	0.02
RSD%	1.83	0.83	0.85

Table 2. Composition of a thin HfO₂ film on Si

	Total Si ⁴⁺ at%	Total Hf at%	Total O at%	Total C at%*	Uncorrected O:Hf ratio
Avg.	4.6	20.5	60.1	14.9	2.93
Std. Dev. (1σ)	0.11	0.24	0.37	0.56	-
RSD%	2.3	1.2	0.6	3.8	-

* Approximately 75% of the carbon is adsorbed C ('adventitious' C) on the surface and not in the layer. The remainder is within the film and/or the interface.

Figure 1. Schematic of HfO₂ film on Si substrate

Composition and stoichiometry of HfO₂ films can vary greatly depending on the process (i.e. MOCVD vs. ALD). Furthermore, the stoichiometry is not simply a measure of total O to total Hf concentrations. All thin HfO₂ films have some O associated with the interfacial layer that is not a part of the HfO₂ layer. In addition, all deposited films have surface-adsorbed O (in the form of carbon-oxygen functionalities, OH bonds, or H₂O) that is also not part of the HfO₂ film. Therefore a careful accounting of O as HfO₂ and non-HfO₂ composition is required to produce a meaningful O:Hf stoichiometry value. The third column in Table 1 shows the O:Hf stoichiometry corrected for O bonded to non-Hf species, whereas Table 2 shows the composition in atomic %. Again, the values in the tables are averages from multiple measurements on a single wafer. The total O:Hf ratio from the atomic concentrations is considerably higher than the corrected O:Hf ratio shown in Table 1. The excess O (Table 2) can be attributed to interfacial oxide, and surface-adsorbates, as noted above.

The corrected O:Hf ratio (Table 1) is higher than the theoretical value of '2' for HfO₂. While the calculated value for the corrected ratio is often 2 on many samples, the value of 2.5 on this film suggests that the film is O enriched.

As previously mentioned, determining the uniformity of the film thicknesses and compositions can be critical for process control. Figure 2 illustrates the capability of the HfO₂ *High Precision XPS Measurement* to determine uniformity of interfacial layer thickness, HfO₂ thickness and O:Hf ratio from a radial scan across a wafer. In this example, these parameters are uniform across the wafer.

The development of the HfO₂ *High Precision XPS Measurement* provides a single rapid acquisition and precise analysis that can yield critical information about HfO₂ dielectric films. This analysis provides a highly repeatable measurement of the thickness of the HfO₂ layer, the thickness of the interfacial layer, total film stack thickness (HfO₂ layer + interfacial layer), composition of the dielectric layer plus the interfacial layer, and the stoichiometry coefficient of the HfO₂ film.

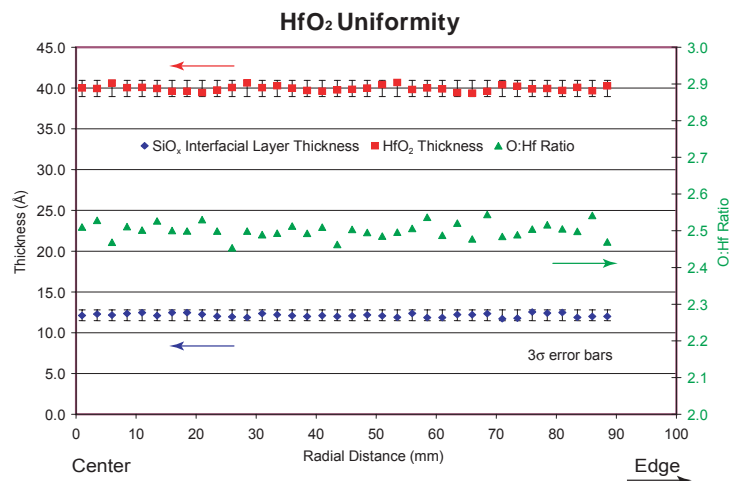


Figure 2. Uniformity of layer thickness and stoichiometry across a HfO₂ film on a Si wafer

United States Locations

Tempe, Arizona
+1 480 239 0602 info.az@eaglabs.com
+1 602 470 2655 fax

Sunnyvale, California
810 Kifer Road
+1 408 530 3500 info.ca@eaglabs.com
+1 408 530 3501 fax

1135 E Arques Avenue
+1 408 738 3033
+1 408 738 3035 fax

785 Lucerne Drive
+1 408 737 3892
+1 408 737 3916 fax

Peabody, Massachusetts
+1 978 278 9500 info.ma@eaglabs.com
+1 978 278 9501 fax

Chanhassen, Minnesota
+1 952 828 6411 info.mn@eaglabs.com
+1 952 828 6449 fax

East Windsor, New Jersey
+1 609 371 4800 info.nj@eaglabs.com
+1 609 371 5666 fax

Syracuse, New York
+1 315 431 9900 info.ny@eaglabs.com
+1 315 431 9800 fax

Raleigh, North Carolina
+1 919 829 7041 info.nc@eaglabs.com
+1 919 829 5518 fax

Round Rock, Texas
+1 512 671 9500 info.tx@eaglabs.com
+1 512 671 9501 fax

International Locations

Shanghai, China
+ 86 21 6879 6088 info.cn@eaglabs.com
+ 86 21 6879 9086 fax

Tournefeuille, France
+ 33 5 61 73 15 29 info.fr@eaglabs.com
+ 33 5 61 73 15 67 fax

Frankfurt, Germany
+ 49 (0) 693053213 info.de@eaglabs.com
+ 49 (0) 69307941 fax

Tokyo, Japan
+ 81 3 5396 0531 info.jp@eaglabs.com
+ 81 3 5396 1930 fax

HsinChu, Taiwan
+ 886 3 5632303 info.tw@eaglabs.com
+ 886 3 5632306 fax

Uxbridge, United Kingdom
+ 44 (0) 1895 811194 info.uk@eaglabs.com
+ 44 (0) 1895 810350 fax