Measurement of Thicknesses of High-κ Gate-Dielectric Films on Silicon

Materials with high dielectric constants such as HfO_2 (hafnium oxide), ZrO_2 (zirconium oxide), $HfSiO_4$ (hafnium silicate) and $ZrSiO_4$ (zirconium silicate) are expected to be used as "high-κ" gate oxides in future semiconductor devices. The gate oxides will be thin films having thicknesses of several nanometers, but the physical thickness will be larger than those of SiO_2 or SiON (silicon oxynitride) in current gate-oxide layers since the new materials have higher dielectric constants than SiO_2 or SiON. In this way, planned reductions in feature sizes of next-generation devices can be achieved. While many techniques have been used to measure and monitor thin-film thicknesses on the nanometer scale, X-ray photoelectron spectroscopy (XPS) has been shown to provide the needed accuracy and sensitivity. Thickness measurements by XPS, however, depend on knowledge of a material parameter, the effective attenuation length (EAL), for the relevant photoelectron energy and the particular measurement configuration. We have calculated EALS for candidate high-κ dielectrics using a new NIST Database for the Simulation of Spectra for Surface Analysis (SESSA).

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X-ray photoelectron spectroscopy (XPS) has the required sensitivity and accuracy to measure and monitor thin-film thicknesses on the nanometer scale, however the thickness measurements depend upon the knowledge of the effective attenuation lengths (EALs). NIST researchers have calculated EALs for thin films of HfO_2, ZrO_2, $HfSiO_4$, and $ZrSiO_4$ on silicon in a common XPS measurement configuration. The EALs differ from the corresponding electron inelastic mean free paths (IMFPs) on account of elastic scattering of the photoelectrons in the sample. While the IMFP is a material parameter, the EAL can vary with film thickness and electron-emission angle.

The figure shows an example of our results. The ratio of the EAL, L, for substrate Si 2p photoelectrons excited by Al Kα x-rays in an overlayer film of HfO_2 to the IMFP, λ_i, in HfO_2 is plotted as a function of film thickness. The IMFP for Si 2p photoelectrons excited by Al Kα x-rays in HfO_2 is 2.17 nm (from a NIST-developed predictive equation for IMFPs). EALs for specific HfO_2 film thicknesses and photoelectron emission angles can be obtained from the ratios plotted in the Figure. Qualitatively similar results were obtained for ZrO_2, $HfSiO_4$, and $ZrSiO_4$.

NIST issued an Electron Effective-Attenuation-Length Database (SRD 82) in 2001. This database provided EALs that were computed from an algorithm based on the so-called transport approximation in which it is assumed that the electron-scattering properties in film and substrate materials are similar. Until SESSA was developed, however, it was not possible to determine uncertainties associated with use of the transport approximation. For HfO_2, the differences between EALs from SRD 82 and SESSA were typically less than 5 % although the differences could be as much as 20 % for an emission angle of 80^{o}. Comparisons of EALs from SRD 82 with experimental measurements have shown generally satisfactory agreement.

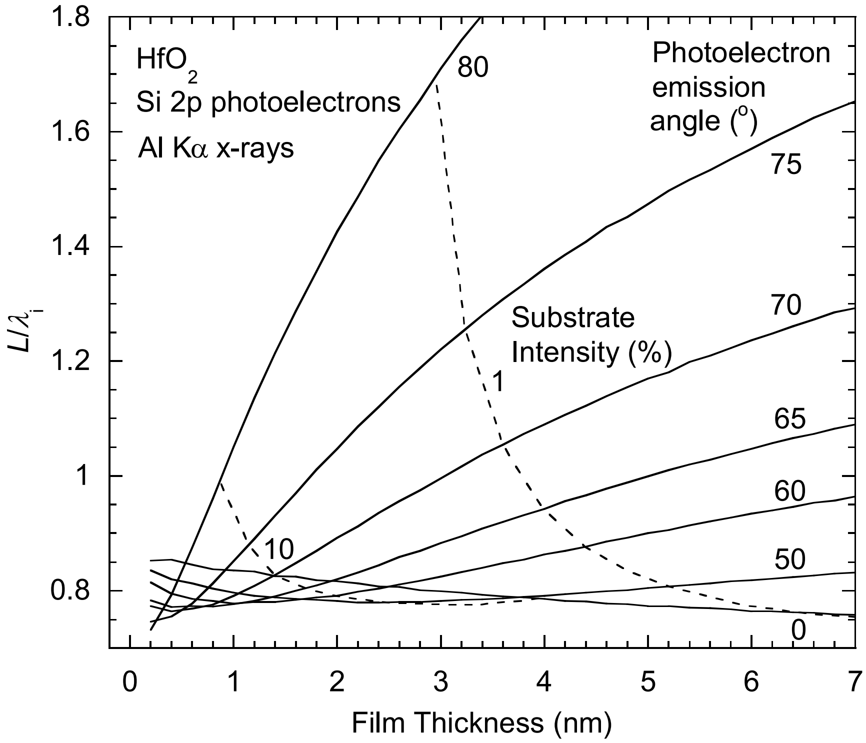
The new NIST Database for the Simulation of Spectra for Surface Analysis (SESSA), SRD 82, contains extensive data for the many parameters needed in quantitative XPS (as well as for the companion technique of Auger electron spectroscopy) and can simulate XPS spectra for layered samples using a very efficient Monte Carlo algorithm.

Future Plans: **NIST researchers are calculating ratios of Si 2p and Hf 4f photoelectron intensities as a function of HfO_2 thickness for various experimental conditions. These "calibration curves" should provide a simple and convenient means to determine film thickness in comparisons with experimental measurements. We are also collaborating with D.W. Moon of the Korea Research Institute of Standards and Science to make EAL measurements on well-characterized films of HfO_2 on Si.**

Publications:

C. J. Powell, A. Jablonski, W. S. M. Werner, and W. Smekal, ***"Characterization of Thin Films on the Nanometer Scale by Auger Electron Spectroscopy and X-ray Photoelectron Spectroscopy,"*** Appl. Surf. Science **239**, 470 (2005).

C. J. Powell, W. Smekal, and W. S. M. Werner, ***"A New NIST Database for the Simulation of Electron Spectra for Surface Analysis (SESSA): Application to Angle-Resolved X-Ray Photoelectron Spectroscopy of HfO_2, ZrO_2, $HfSiO_4$, and $ZrSiO_4$ Films on Silicon,"*** in *Characterization and Metrology for ULSI Technology 2005*, D. G. Seiler et al., eds., AIP Conference Proceedings 788 (American Institute of Physics, Melville, 2005), p. 107.



The solid lines show ratios of the EAL, *L*, to the IMFP, λ_i, as a function of HfO_2 film thickness for XPS with Al Kα x-rays and a common XPS configuration. The dashed lines show this ratio for film thicknesses for which the substrate Si 2p photoelectron intensity was reduced to 1 % and 10 % of its original value.