# Effects of Elastic Scattering and Analyzer-Acceptance Angle on the Analysis of Angle-Resolved XPS Data

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## INTRODUCTION

Angle-resolved XPS (ARXPS) is frequently used to obtain information on the variation of composition with depth. Reliable analysis of the experimental data, however, is currently based on the validity of a number of assumptions [1]. We consider here the validity of two of these assumptions, namely the neglect of elastic scattering of the signal electrons and neglect of the finite acceptance angle of the analyzer.

We determined intensities of N 1s, O 1s, Hf 4f, Si (oxide) 2p, and Si (substrate) 2p peaks at selected emission angles for $SiO_{1.6}N_{0.4}$ and $HfO_{1.9}N_{0.1}$ films on Si with various thicknesses. The intensities were calculated using the NIST Database for Simulation of Electron Spectra for Surface Analysis (SESSA) [2], an efficient XPS simulation tool [3]. Simulations were performed with Al Kα X-rays (and film thicknesses of 5 Å, 15 Å, 25 Å, 35 Å, and 45 Å) and Cu Kα X-rays (and film thicknesses of 25 Å, 75 Å, 125 Å, 175 Å, and 225 Å), sample tilting, and differential elastic-scattering cross sections from the relativistic partial-wave expansion method (Mott cross sections). We also performed simulations with the straight-line approximation (SLA) in which elastic scattering is neglected.

Peak intensities were compared for four models:

(a) Mott cross sections and an analyzer semi-angle of 12°
(b) Mott cross sections and a semi-angle of 0.5°
(c) SLA and a semi-angle of 12°
(d) SLA and a semi-angle of 0.5°

References

[1] P. J. Cumpson, J. Electron Spectrosc. Relat. Phenom. 73, 25 (1995).
[2] http://www.nist.gov/srd/nist100.htm.
[3] W. Smekal, W. S. M. Werner, and C. J. Powell, Surf. Interface Anal. 37, 1059 (2005).
[4] W. S. M. Werner, Surf. Interface Anal. 31, 141 (2001).
[5] C. J. Powell, W. S. M. Werner, and W. Smekal, Appl. Phys. Letters 89, 172101 (2006).
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## DESCRIPTION of SESSA [2,3]

SESSA provides data for the parameters needed for quantitative Auger AES and XPS. SESSA can also perform Monte Carlo simulations of AES and XPS spectra for multi-layered thin-film samples based on partial-intensity analysis [4] and an optimized simulation algorithm [3]. In these simulations, elastic scattering can be switched "on" or "off" (i.e., the SLA).

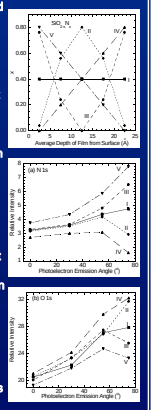
## NEW VERSION of SESSA (fall, 2009)

SESSA Version 1.2 is expected to be released in fall, 2009. This version will include the capability to perform XPS simulations with various amounts of X-ray polarization (both linear and circular). SESSA 1.2 will be useful for XPS applications with synchrotron radiation.

## SESSA SIMULATIONS for 25 Å SiON FILMS on Si with VARYING N COMPOSITION PROFILES with DEPTH [5]

We have previously used SESSA to determine N 1s and O 1s peak intensities for a 25 Å $SiO_{2-x}N_x$ film with different N composition profiles with depth. Common ARXPS conditions were assumed (Al Kα X-rays, sample tilting, angle of 55° between the direction of X-rays and the analyzer direction).

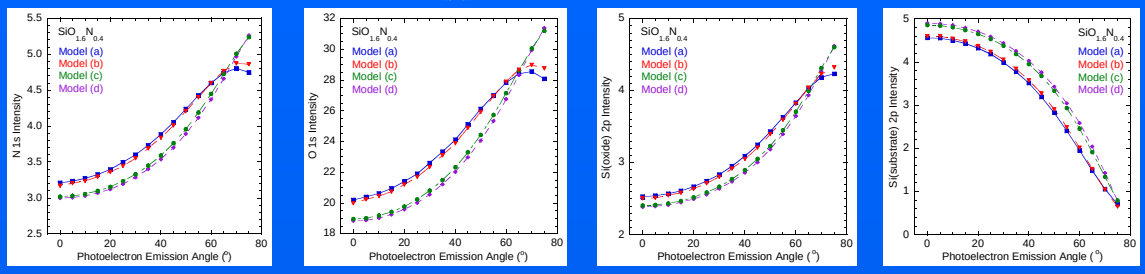
Plots of the N 1s and O 1s peak intensities as a function of photoelectron emission angle show similar trends. The N 1s plots differ significantly only for the 75° emission angle (with respect to the surface normal). This emission angle, however, is outside the range for which a constant attenuation length might reasonably be assumed to be valid in the analysis of the ARXPS data [6]. At the other three emission angles, much smaller relative differences are found, and it is likely that only linear increases or decreases of N concentration with depth would be distinguishable from the other three distributions (for the present high assumed N dose and high dose variation.



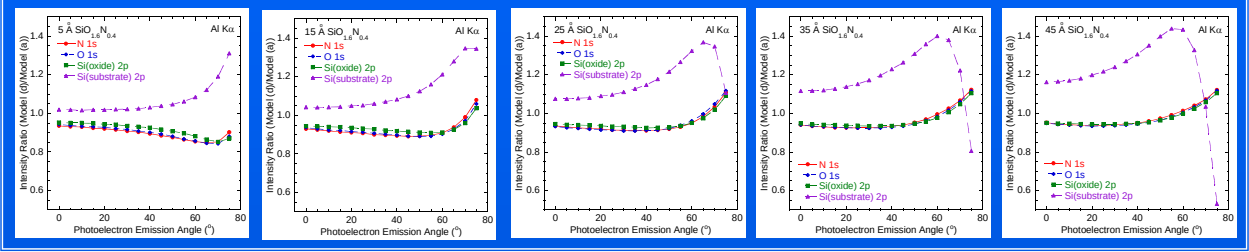
The relative changes of the O 1s intensities are smaller than those for the N 1s intensities, but the largest dispersion also occurs for the 75° emission angle. Insignificant changes occurred in the Si (substrate) and Si (oxide) 2p intensities for the different N profiles.

## $SiO_{1.6}N_{0.4}$ FILMS on Si (Al Kα X-rays)

Plots of N 1s, O 1s, Si (oxide) 2p, and Si (substrate) 2p intensities for a 25 Å $SiO_{1.6}N_{0.4}$ film on Si as a function of photoelectron emission angle.

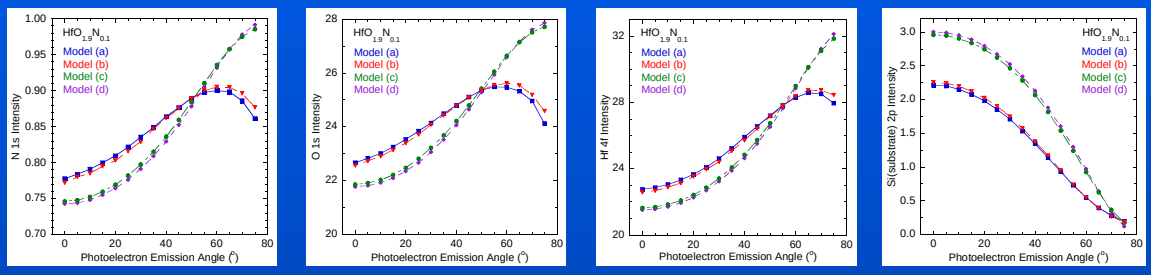


Ratios of peak intensities from Model (d) to Model (a) for each line as a function of photoelectron emission angle for different $SiO_{1.6}N_{0.4}$ film thicknesses.

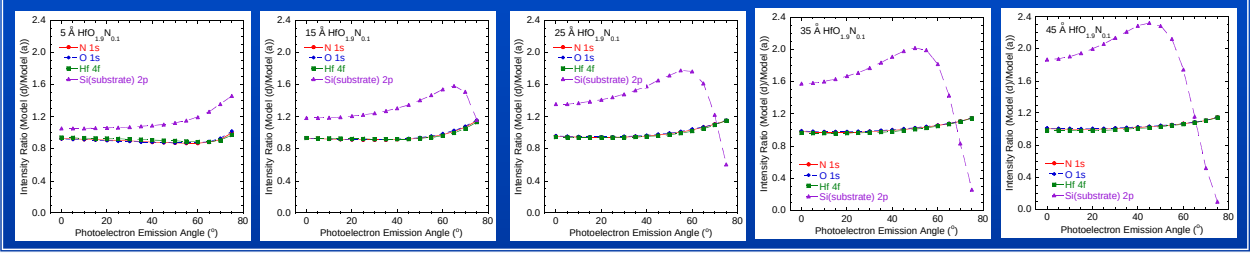


## $HfO_{1.9}N_{0.1}$ FILMS on Si (Al Kα X-rays)

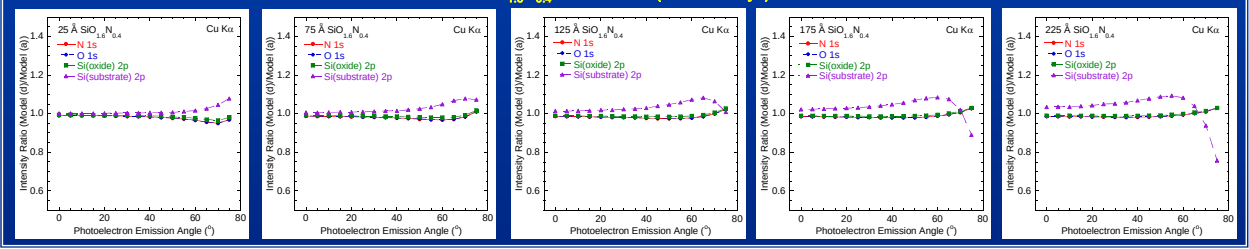
Plots of N 1s, O 1s, Hf 4f, and Si (substrate) 2p intensities for a 25 Å $HfO_{1.9}N_{0.1}$ film on Si as a function of photoelectron emission angle.



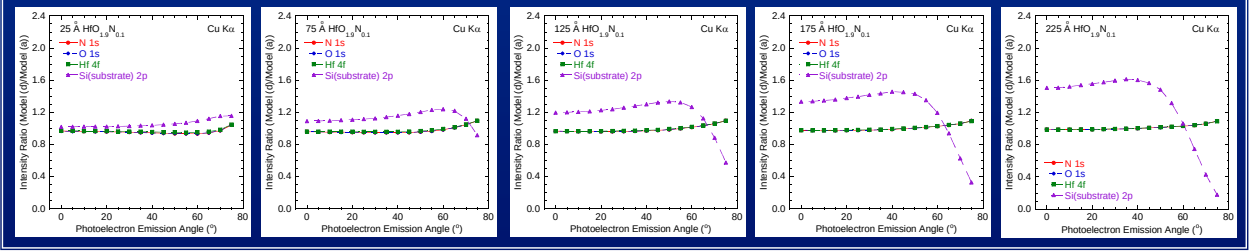
Ratios of peak intensities from Model (d) to Model (a) for each line as a function of photoelectron emission angle for different $HfO_{1.9}N_{0.1}$ film thicknesses.

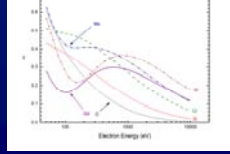


## $SiO_{1.6}N_{0.4}$ FILMS on Si (Cu Kα X-rays)



## $HfO_{1.9}N_{0.1}$ FILMS on Si (Cu Kα X-rays)



## SUMMARY

- SESSA simulations for various thicknesses of $SiO_{1.6}N_{0.4}$ and $HfO_{1.9}N_{0.1}$ films on Si show that inclusion of elastic scattering leads to substantial changes in peak intensities as a function of emission angle. Changes in the analyzer acceptance semi-angle led to smaller changes in peak intensities. The intensity changes due to inclusion of elastic scattering are comparable to those resulting from the different N composition profiles shown at left.
- Ratios of peak intensities for Model (d) (elastic scattering off, small analyzer acceptance angle) to Model (a) (elastic scattering on, finite analyzer angle) as a function of emission angle show clearly the lack of validity of the simplifying assumptions made in conventional analyses of ARXPS data. In particular, the ratios for the Si (substrate) 2p intensity change appreciably with emission angle. Simple replacement of the inelastic mean free path by an effective attenuation length does not appear to be reliable, even for emission angles between 0° and 55° [6].
- Elastic-scattering effects are stronger in $HfO_{1.9}N_{0.1}$ than $SiO_{1.6}N_{0.4}$, as expected. The single-scattering albedo $\omega$ (the ratio of the inelastic mean free path (IMFP) to the sum of the IMFP and the transport mean free path) is a convenient measure of the strength of elastic scattering in XPS. The plot at right shows $\omega$ as a function of electron energy for six illustrative elemental solids [C. J. Powell and A. Jablonski, to be published]. The value of $\omega$ for Si (substrate) 2p, Hf $4f_{7/2}$, O 1s, and N 1s photoelectrons excited by Cu Kα X-rays in $HfO_{1.9}N_{0.1}$ is approximately 0.13, a value comparable to $\omega$ for Si (substrate) 2p, Si (oxide) 2p, O 1s, and N 1s photoelectrons excited by Al Kα X-rays in $SiO_{1.6}N_{0.4}$ (between 0.11 and 0.15).