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Characterization of thin films on the nanometer scale by Auger electron spectroscopy and X-ray photoelectron spectroscopy

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Abstract

We describe two NIST databases that can be used to characterize thin films from Auger electron spectroscopy (AES) and X-ray photoelectron spectroscopy (XPS) measurements. First, the NIST Electron Effective-Attenuation-Length Database provides values of effective attenuation lengths (EALs) for user-specified materials and measurement conditions. The EALs differ from the corresponding inelastic mean free paths on account of elastic-scattering of the signal electrons. The database supplies "practical" EALs that can be used to determine overlayer-film thicknesses. Practical EALs are plotted as a function of film thickness, and an average value is shown for a user-selected thickness. The average practical EAL can be utilized as the "lambda parameter" to obtain film thicknesses from simple equations in which the effects of elastic-scattering are neglected. A single average practical EAL can generally be employed for a useful range of film thicknesses and for electron emission angles of up to about 60°. For larger emission angles, the practical EAL should be found for the particular conditions. Second, we describe a new NIST database for the Simulation of Electron Spectra for Surface Analysis (SESSA) to be released in 2004. This database provides data for many parameters needed in quantitative AES and XPS (e.g., excitation cross-sections, electron-scattering cross-sections, lineshapes, fluorescence yields, and backscattering factors). Relevant data for a user-specified experiment are automatically retrieved by a small expert system. In addition, Auger electron and photoelectron spectra can be simulated for layered samples. The simulated spectra, for layer compositions and thicknesses specified by the user, can be compared with measured spectra. The layer compositions and thicknesses can then be adjusted to find maximum consistency between simulated and measured spectra, and thus, provide more detailed characterizations of multilayer thin-film materials. SESSA can also provide practical EALs, and we compare values provided by the NIST EAL database and SESSA for hafnium dioxide. Differences of up to 10% were found for film thicknesses less than 20 Å due to the use of different physical models in each database.

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1. Introduction

Auger electron spectroscopy (AES) and X-ray photoelectron spectroscopy (XPS) have been extensively used for determining the chemical compositions of thin films of nanometer thicknesses in a large variety of applications and for observing any compositional changes following fabrication, processing, and exposure to the service environment. It is also frequently desired in these applications to measure film thicknesses and changes of these thicknesses with time or following processing. While AES and XPS are ideal for these applications in which they have surface sensitivities on the nanometer scale, it has until recently been difficult to obtain the desired information with reasonable reliability and simplicity.

Two NIST databases, the NIST Electron Effective-Attenuation-Length Database [1] and the NIST database for Simulation of Electron Spectra for Surface Analysis (SESSA) [2], can be used to characterize nanometer-films by AES and XPS. We describe these two databases and give examples of their use in Sections 2 and 3, respectively. A comparison of results from these databases for the measurement of thicknesses of hafnium dioxide films on a silicon substrate is presented in Section 4. We conclude with a summary in Section 5.

2. NIST Electron Effective-Attenuation-Length Database

The NIST Electron Effective-Attenuation-Length Database (SRD 82) [1] was first issued in 2001. This database provides values of electron effective attenuation lengths (EALs) for solid elements and compounds at user-selected electron energies between 50 and 2000 eV. The database was designed mainly to provide EALs (to account for effects of elastic-scattering of the signal electrons) for applications in AES and XPS [3,4]. For these applications, EALs are needed mainly for the measurement of thicknesses of overlayer-films and, to a much lesser extent, for measurements of the depths of thin marker layers [3,4].

The EALs (and other functions and parameters listed below) provided by SRD 82 are calculated from analytical expressions derived from solution of the Boltzmann kinetic equation within the transport approximation [5] for measurement conditions supplied by the user [3,4]. This algorithm accounts for elastic-scattering along the trajectories of the signal electrons in the solid. Two material properties are needed for the EAL calculation: (a) the inelastic mean free path (IMFP), λ_i, for the signal electrons, and (b) the transport mean free path (TMFP), λ_t, that is a measure of the strength of large-angle elastic-scattering of the signal electrons. IMFP and TMFP values are derived for a user-specified material composition from data provided in two NIST databases [6,7]. For XPS, it is necessary for users to supply values of the photoionization asymmetry parameter [8].

SRD 82 supplies ‘‘local’’ EALs (derived from the local slope of the calculated emission depth distribution function (DDF) at a user-specified depth) and ‘‘practical’’ EALs suitable for measurements of overlayer-film thicknesses or depths of thin marker layers. For the most common application, measurement of overlayer-film thicknesses, the practical EAL, L, can be defined as follows:

$$L = \frac{t}{\cos\alpha(\ln I_0^s - \ln I_t^s)} \tag{1}$$

where α is the electron emission angle with respect to the sample normal, and I_0^s and I_t^s are the substrate-signal intensities before and after deposition of an overlayer-film of thickness t [3,4]. The practical EAL is thus a function of α and t as well as of the IMFP and TMFP; it also depends on the instrumental configuration and whether the signal electrons are Auger electrons or photoelectrons [3,4].

The accuracy of the algorithm used for the EAL calculations in SRD 82 was recently assessed from comparisons of EALs for a group of photoelectron lines in Si, Cu, and Au with corresponding values obtained from Monte Carlo simulations [9]. It was found that the average difference in the computed EALs was 5.0% for these lines with an angle, ψ, between the direction of the X-rays and the direction of the analyzer of 54° and with emission angles between 0° and 80°. We also point out a key assumption in the model on which SRD 82 is based, namely, that the elastic- and inelastic-scattering properties of the overlayer-film are similar to those of the substrate [4]. The validity of this assumption will be discussed in Section 3.