The NIST Electron Effective-Attenuation-Length Database

C. J. Powell and A. Jablonski[1]

Surface and Microanalysis Science Division, National Institute of Standards and Technology, Gaithersburg, MD 20899-8370, USA
[1]Institute of Physical Chemistry, Polish Academy of Sciences, ul. Kasprzaka 44/52, 01-224 Warsaw, Poland

(Received November 19, 2001; accepted February 6, 2002)

The NIST Electron Effective-Attenuation-Length Database provides values of electron effective attenuation lengths (EALs) in solid elements and compounds at selected electron energies between 50 eV and 2,000 eV. The database was designed mainly to provide EALs (to account for effects of elastic-electron scattering) for applications in surface analysis by Auger-electron spectroscopy (AES) and X-ray photoelectron spectroscopy (XPS). For these applications, EALs are needed mainly for measurements of the thicknesses of overlayer films and to a much lesser extent for measurements of the depths of thin marker layers. EALs are calculated using an algorithm based on electron transport theory for measurement conditions specified by the user. The database also provides values of other parameters needed for other quantitative applications of AES and XPS.

1. Introduction

The attenuation length (AL) and the more recent equivalent term effective attenuation length (EAL) are frequently used in the literature on Auger-electron spectroscopy (AES) and X-ray photoelectron spectroscopy (XPS). These terms generally refer to the rate at which AES and XPS signal intensities from a substrate material or an overlayer material change as a function of overlayer-film thickness. In most early work, these intensities were found to vary nearly exponentially with film thickness and the exponential parameter was referred to as the attenuation length. This parameter was also thought to be identical to the inelastic mean free path (IMFP) for the particular material and electron energy.

It is now known that elastic-electron scattering can modify the trajectories of signal electrons in AES and XPS. As a result, these electrons do not travel along straight-line paths from their point of generation to the sample surface. It is therefore inappropriate to refer to the exponential parameter in the overlayer-film experiments as the AL [1]. The term effective attenuation length is now recommended for this purpose [2]. As a result of elastic scattering, the EAL is generally different from the corresponding IMFP.

The present recommended definition of the EAL [1-3] is relevant to measurements of the depth of a thin marker layer (or δ-layer) near a surface. Measurements of overlayer-film thicknesses, however, are based on changes of AES and XPS intensities with film thickness, and it is necessary to modify the EAL definition for this application [4]. For both applications, the EAL can be defined in terms of the local slope of the emission depth distribution function [1-3] (for the depth of the marker layer) or of an integral of this function (for the overlayer-film thickness); these EALs are referred to as local EALs.

It is more useful, however, to define practical EALs in terms of the average slope of the emission depth distribution function (from the surface to the depth of interest) or of the average slope of the integral of this function (for zero overlayer thickness to some thickness of interest) [4]. These practical EALs can be used with equations derived on the assumption that elastic-electron scattering is not significant to determine overlayer-film thicknesses (the most common application) or marker-layer depths. It should be emphasized, however, that the practical EALs are based on the implicit assumption that the emission depth distribution function and its integral are exponential functions even if they are not. The practical EALs are thus empirical parameters for the particular conditions (e.g., overlayer-film thickness, electron emission angle, and experimental configuration for XPS).

Version 1.0 of the NIST Electron Effective-Attenuation-Length Database (SRD 82) is now available [5]. While the database provides local and practical EALs for measurements of overlayer-film thicknesses and of marker-layer depths, the practical EALs for measurement of overlayer-film thicknesses will likely be of greatest interest for most AES and XPS applications. These practical EALs can differ from the corresponding IMFPs by up to about 35 % for common AES and XPS measurement conditions.

We give here a brief description of the NIST EAL Database and an example of its use.

2. NIST Electron Effective-Attenuation-Length Database [5]

The EALs (and other functions and parameters listed below) are calculated from analytical expressions derived from solution of the kinetic Boltzmann equation within the transport approximation [6]. Examples of EALs obtained by this approach are described in recent publications [4,7-9]. The EALs depend on two material-dependent parameters, the IMFP and the transport mean free path (TMFP). The EAL Database contains data from the NIST Electron IMFP Database [10] (for IMFPs) and from the NIST Electron Elastic-Scattering Cross-Section Database [11] (for elemental TMFPs). The TMFPs for compounds are computed from the weighted TMFPs for the constituent elements [12]. In addition, the EALs for XPS depend on the photoionization asymmetry parameter [13].

The user will first specify values for certain initial parameters (including the material of interest (element, inorganic compound, or organic compound), the electron energy, the photoionization asymmetry parameter (for XPS), a particular source of IMFP data from the NIST IMFP Database, and the experimental configuration). The user can then choose to obtain local or practical EALs, and will then typically generate a Table of EAL values for selected overlayer-film thicknesses or marker-layer depths; these EAL values can be stored, if desired, for further analysis. The EALs are then displayed on the screen as a function of film thickness or marker depth, and compared with the IMFP. By clicking on the screen, a user can select a particular thickness or depth of interest, and the EAL for that thickness or depth will be displayed together with the percentage attenuation of an assumed substrate-electron signal (for an overlayer) or the percentage attenuation of the marker-layer signal will be displayed for the selected thickness or depth, respectively.

As just indicated, the EAL is typically a function of overlayer thickness (or marker-layer depth). For emission angles less than about 60° (with respect to the surface normal) and for overlayer-film thicknesses of practical relevance in AES and XPS measurements, however, the practical EAL does not vary appreciably with overlayer thickness or emission angle [4,7-9,14]. The database can provide an average practical EAL for a selected film thickness (or marker depth) at the specified emission angle. This average practical EAL can be used as the "lambda parameter" in measurements of overlayer-film thicknesses by AES and XPS [4,7-9]. For emission angles larger than about 60°, it will often be necessary to obtain a practical EAL for an estimated overlayer-film thickness so that a more accurate film thickness can be determined by iteration.

The database can also supply values of certain other parameters for an infinitely thick material: the electron mean escape depth [7], the EAL for quantitative analysis by AES and XPS [4], the correction parameters Q_x and β_{eff}

for XPS [15,16], and the correction parameter Q_A for AES [15,16]. In addition, the database supplies the average EAL for elemental solids from the CS2 EAL estimation formula proposed by Cumpson and Seah [14].

The database has two further options. First, the user can obtain values of the emission depth distribution function (DDF) for a specified material and electron energy. This DDF can be visually compared with the DDF obtained when elastic-electron scattering was neglected. Second, the user can obtain values of the correction factor (CF), the ratio of the DDF with elastic-electron scattering considered to the DDF with elastic-electron scattering neglected [17]. For each of these options, Tables of the DDF and the CF are created and can be stored for later analysis.

It is also possible to make on-screen comparisons of EAL, DDF, or CF data in selected files. These graphical comparisons can be printed and saved in Windows bitmap format for easy incorporation into other documents.

3. Practical EALs (Ag $3d_{5/2}$ Photoelectrons)

As an example of the use of the NIST EAL Database [5], we present plots of the ratio of the practical EAL, L, to the IMFP, λ, in Fig. 1 as a function of overlayer-film thickness for Ag $3d_{5/2}$ photoelectrons excited by Al Kα x-rays for a configuration in which the angle between the axes of the x-ray source and the analyzer, ψ, was 55°. The solid lines show values of this ratio for various values of the electron emission angle, α, with respect to the surface normal. The short-dashed lines in Fig. 1 are loci of constant relative intensity of Ag $3d_{5/2}$ photoelectrons from an assumed Ag substrate. These loci were calculated to show L/λ values corresponding to film thicknesses for which these substrate intensities were 1 %, 2 %, 5 %, and 10 % of the values found for no overlayer film.

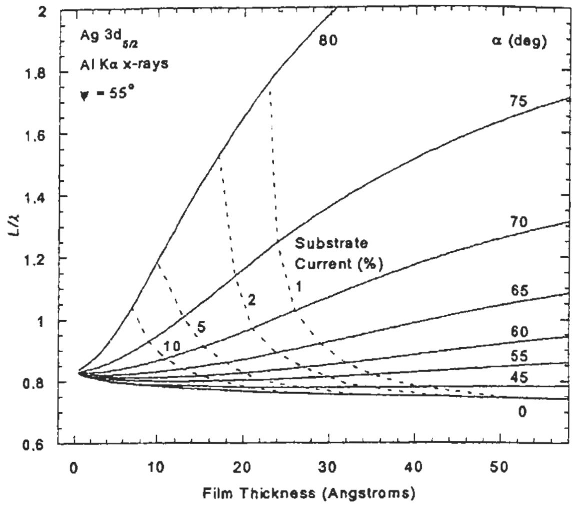

Fig. 1. Plot of the ratio of the practical EAL, L, to the IMFP, λ, for Ag $3d_{5/2}$ photoelectrons (solid lines) as a function of overlayer thickness (for excitation by Al Kα x-rays with an angle ψ between the x-ray source and the analyzer axes of 55°) at different emission angles α. The short-dashed lines show L/λ values for film thicknesses for which the Ag $3d_{5/2}$ photoelectron intensity from an assumed substrate was reduced to 1 %, 2 %, 5 %, and 10 % of the value for the substrate without an overlayer film.

We consider now two ranges of overlayer-film thicknesses in Fig. 1 that are believed to be representative of practical XPS measurements. First, for each α, we obtain the average values, L^1_{ave}/λ, by averaging the L/λ values in Fig. 1 (solid lines) for overlayer-film thicknesses, t, from zero to the value corresponding to attenuation of the substrate intensity to 1 % of its original value for $t = 0$ (Condition A). Second, we obtain similar averages, L^{10}_{ave}/λ, for film thicknesses from zero to the value corresponding to attenuation of the substrate intensity to 10 % of its original value (Condition B).

Figure 2 shows plots of L^1_{ave}/λ and L^{10}_{ave}/λ as a function of emission angle. For 0° α 60°, the L^1_{ave}/λ and L^{10}_{ave}/λ values are of similar magnitude and vary slowly with α. Average values of L can be obtained from these ratios and used as the "lambda parameter" to obtain film thicknesses with the familiar equations derived from the assumption that elastic-electron scattering could be neglected. For emission angles larger than about 60°, the L^1_{ave}/λ and L^{10}_{ave}/λ values in Fig. 2 change more rapidly with α, and

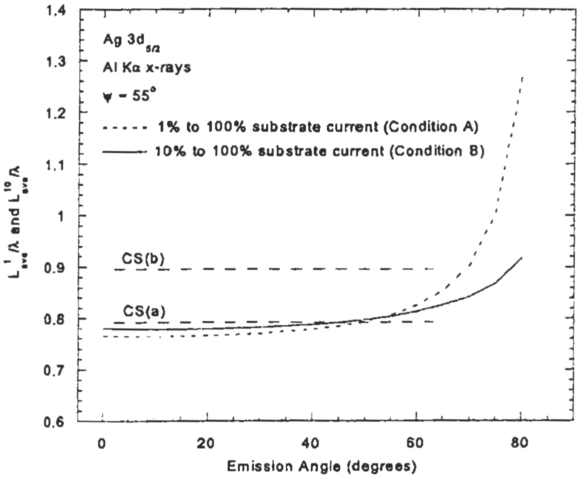

Fig. 2. Plots of L^{1}_{ave} and L^{10}_{ave} for Ag $3d_{5/2}$ photoelectrons (as for Fig. 1) as a function of emission angle, α, for Condition A (solid line) and Condition B (short-dashed line). The long-dashed lines designated CS(a) and CS(b) show EAL results from Cumpson and Seah [14] as described in the text.

values of L should be obtained for specific values of α and t (e.g., from the solid lines in Fig. 1). In such cases, it may be necessary to estimate a film thickness, determine L for this thickness, and then refine the film thickness by iteration.

For α 60°, our EALs are in good agreement with EALs derived from the Monte Carlo simulations of Cumpson and Seah [14], designated CS(a) in Fig. 2. There is poorer agreement (as expected) with results from their more approximate predictive EAL formula (their CS2 formula), designated CS(b) in Fig. 2.

Acknowledgments

One of the authors (CJP) wishes to acknowledge partial support from the NIST Standard Reference Data Program and the other author (AJ) wishes to acknowledge partial support by KBN Grant 2P03B 039 18.

References

[1] W. H. Gries and W. Werner, Surf. Interface Anal. **16**, 149 (1990).

[2] A. Jablonski and C. J. Powell, J. Electron Spectrosc. Relat. Phenom. **100**, 137 (1999).

[3] ISO 18115: 2001. Surface chemical analysis – Vocabulary, International Organization for Standardization, Geneva, 2001; Standard E 673-98, Annual Book of ASTM Standards, Vol. 3.06, American Society for Testing and Materials, West Conshohocken, Pennsylvania, 2001, p. 735.

[4] C. J. Powell and A. Jablonski, Surf. Interface Anal. (in press).

[5] C. J. Powell and A. Jablonski, NIST Electron Effective-Attenuation-Length Database (SRD 82), Version 1.0, National Institute of Standards and Technology, Gaithersburg, Maryland, 2001.

[6] I. S. Tilinin, A. Jablonski, J. Zemek, and S. Hucek, J. Electron Spectrosc. Relat. Phenom. **87**, 127 (1997).

[7] C. J. Powell and A. Jablonski, J. Electron Spectrosc. Relat. Phenom. **114-116**, 1139 (2001); ibid. 107, 201 (2000).

[8] C. J. Powell and A. Jablonski, Surf. Science **488**, L547 (2001).

[9] C. J. Powell and A. Jablonski, J. Vac. Sci. Tech. A **19**, 2604 (2001).

[10] C. J. Powell and A. Jablonski, NIST Electron Inelastic-Mean-Free-Path Database (SRD 71), Version 1.1, National Institute of Standards and Technology, Gaithersburg, Maryland, 2001.

[11] A. Jablonski, NIST Electron Elastic-Scattering Cross-Section Database (SRD 64), Version 2.0, National Institute of Standards and Technology, Gaithersburg, Maryland, 2000.

[12] A. Jablonski, Phys. Rev. B **58**, 16470 (1998).

[13] I. M. Band, Yu. I. Kharitonov, and M. B. Trzhaskovskava, At. Data Nucl. Data Tables **23**, 443 (1979).

[14] P. J. Cumpson and M. P. Seah, Surf. Interface Anal. **25**, 430 (1997).

[15] A. Jablonski, Surf. Science **364**, 380 (1996).

[16] A. Jablonski and I. S. Tilinin, J. Electron Spectrosc. Relat. Phenom. **26**, 374 (1995).

[17] A. Jablonski and S. Tougaard, Surf. Interface Anal. **26**, 374 (1998).