NIST Databases for Surface Analysis by Auger-Electron Spectroscopy and X-Ray Photoelectron Spectroscopy

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A brief description is given of four databases issued by the National Institute of Standards and Technology (NIST) for applications in surface analysis by Auger-electron spectroscopy (AES) and x-ray photoelectron spectroscopy (XPS). These databases are: the NIST X-Ray Photoelectron Spectroscopy Database, the NIST Electron Elastic-Scattering Cross-Section Database, the NIST Electron Inelastic-Mean-Free-Path Database, and the NIST Electron Effective-Attenuation-Length Database. The purposes and features of these databases are described, and examples are given of data that can be provided.

INTRODUCTION

Data for many physical parameters are needed for applications in surface analysis by Auger-electron spectroscopy (AES) and x-ray photoelectron spectroscopy (XPS), as pointed out by Sekine *et al.*[1-3]. These applications include identification of chemical state from so-called chemical shifts of Auger-electron and photoelectron lines, correction of matrix effects in quantitative AES and XPS analyses, and correction for the effects of elastic scattering of the signal electrons.

The National Institute of Standards and Technology (NIST) currently offers four databases for applications in surface analysis and surface science[4 - 7]. These databases are intended principally for use with AES and XPS but are also useful for other surface-sensitive spectroscopies in which electron beams are employed, for other analytical applications such as electron-probe microanalysis and analytical electron microscopy, and for other purposes such as electron-beam lithography and radiation physics. The four databases are:

- NIST X-Ray Photoelectron Spectroscopy Database (SRD 20)
- NIST Electron Elastic-Scattering Cross-Section Database (SRD 64)
- NIST Electron Inelastic-Mean-Free-Path Database (SRD 71)
- NIST Electron Effective-Attenuation-Length Database (SRD 82)

The SRD 20 database is available on the internet[7] while the other three databases operate on personal computers[6]. All are available without charge. We give here brief descriptions of these databases and examples of their use.

NIST X-RAY PHOTOELECTRON SPECTROSCOPY DATABASE (SRD 20)

Version 3.3 of SRD 20 was released in early 2003[7]. The internet version of this database (first released in 2000) contains a substantial amount of new data and additional information (for the new data) on the specimen material, the measurement conditions, and the data-analysis procedure for each reported measurement. Table 1 shows the main search and display options of Version 3.3.

Version 3.3 contains over 22,000 line positions, chemical shifts, doublet splittings, and energy separations of photoelectron and Auger-electron spectral lines. For data added since the release of Version 2.0, additional informa-

Table 1. Main search and display options for Version 3.3 of the NIST XPS Database.

Identify unknown spectral lines
Binding energy for a photoelectron line
Kinetic energy for an Auger-electron line
Auger parameter
Doublet separation

Retrieve data for selected elements
Binding energy
Auger kinetic energy
Auger parameter
Doublet separation
Chemical shift
Surface or interface core-level shift
Elemental reference data

Retrieve data for selected compounds
Selected groups of elements
Selected element in a compound
Chemical name
Chemical classes (inorganic, organic, ligand, other)

Display Wagner plot

Retrieve data by scientific citation

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tion is available for each data record. There is an expanded set of descriptive codes that are used to describe general features of the specimen material. Information is given on the specimen temperature (at the time of the XPS measurement) and on methods that may have been used to determine the specimen composition and the surface crystallinity. The x-ray source for the XPS measurement is identified and the overall energy resolution is given. Information is provided on the type of curve-fitting function that may have been used for peak location, the full-width at half-maximum intensity of the peak, whether a background function had been utilized, and the uncertainty of peak location (if this information was given in the data source). Finally, comments are included where necessary to describe specific details of the specimen morphology and processing history. Work is ongoing to provide additional evaluated data for the database.

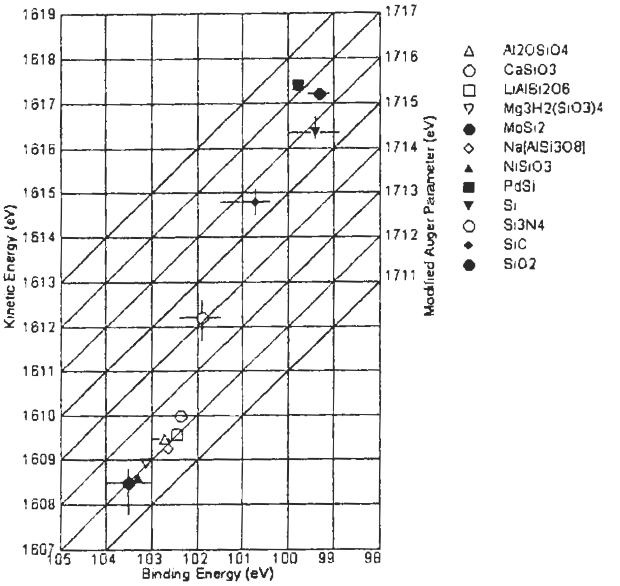

Fig. 1. Wagner plot for silicon and selected silicon compounds prepared by the NIST XPS Database. The same symbols are shown here for some compounds; on the database screen, they are distinguished by different colors.

Figure 1 shows an example of a Wagner plot for Si and a selection of Si compounds that was produced by the database. Such a plot can be very useful in displaying chemical shifts of photoelectron binding energies, Auger-electron kinetic energies, and Auger parameters[8,9].

NIST ELECTRON ELASTIC-SCATTERING CROSS-SECTION DATABASE (SRD 64)

Version 3.0 of SRD 64 was released in December, 2002 [6]. This database provides values of differential elastic-scattering cross sections, total elastic-scattering cross sections, phase shifts, and transport cross sections for elements with atomic numbers from 1 to 96 and for electron energies between 50 eV and 300 keV (in steps of 1 eV). The differential cross sections were calculated using the Dirac partial-wave analysis described by Walker[10]. The scattering potential was obtained from the self-consistent Dirac-Hartree-Fock (DHF) charge density for free atoms [11] with the local exchange potential of Furness and McCarthy[12]. The numerical calculations were performed with the algorithm described by Salvat and Mayol[13]. Further details are given elsewhere[14].

The software for SRD 64 has the following features:

- Graphical display of differential elastic-scattering cross sections in different coordinate systems
- Graphical display of the dependence of transport cross sections on electron energy

- Display of numerical values of differential elastic-scattering cross sections, total elastic-scattering cross sections, and transport cross sections
- Creation of files containing differential elastic-scattering cross sections for specified elements, energies and coordinates
- Creation of files containing plots of differential elastic-scattering cross sections versus scattering angle for one or more elements or for one or more electron energies
- Creation of files containing phase shifts for specified elements and for energies up to 20,000 eV
- Creation of files containing transport cross sections for specified elements and energies
- Creation of random number generators providing the polar scattering angles to be used in Monte Carlo simulations of electron transport in solids; and
- Runs of the random number generators providing the polar scattering angles.

As an example, Fig. 2 shows differential elastic-scattering cross sections for gold as a function of scattering angle at 50 eV, 100 eV, 200 eV, and 500 eV. Cross sections from the database can be compared on a screen, as shown, and printed or stored for future use.

Knowledge of elastic-scattering effects is important for the development of theoretical models for quantitative analysis by AES, XPS, electron microprobe analysis, and analytical electron microscopy. The software package of SRD 64 is designed to facilitate simulations of electron transport for these and similar applications in which electron energies from 50 eV to 300 keV are utilized.

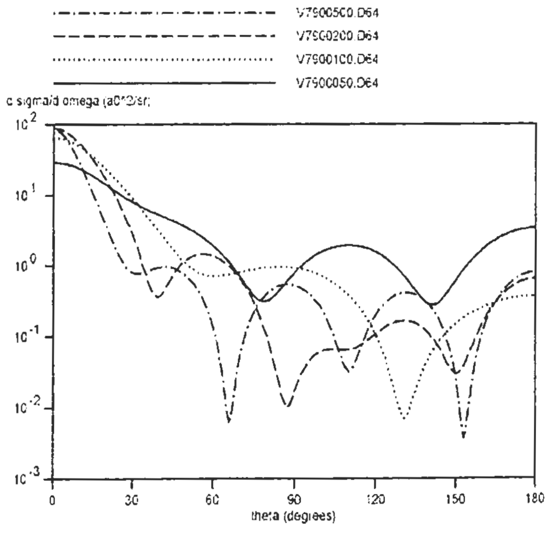

Fig. 2. Comparison of differential elastic-scattering cross sections of gold at electron energies of 50 eV (solid line), 100 eV (dotted line), 200 eV (dashed line), and 500 eV (dot-dashed line) from Version 3.0 of the NIST Electron Elastic-Scattering Cross-Section Database.

Differential cross sections for elastic scattering have often been calculated from the DHF atomic potential (as in Version 3.0 of SRD 64) or the Thomas-Fermi-Dirac potential (as in Versions 1.0 and 2.0 of SRD 64), although cross sections from the DHF potential are considered to be more accurate[14]. Differential cross sections from these two potentials have been frequently used in simulations of signal-electron transport for AES and XPS applications (amongst many others). A comparison has recently been made of differential cross sections from the TFD and DHF potentials as well as of quantities derived from them relevant to AES and XPS (elastic-backscattered intensities for a thin film on a substrate, electron inelastic mean free paths obtained from elastic-peak electron-spectroscopy measurements, and mean escape depths for AES and XPS)[14].

Version 3.0 of SRD 64 provides values of transport cross sections. These cross sections are useful in AES and XPS for calculation of effective attenuation lengths (needed for the determination of overlayer-film thicknesses)[15 - 17], for calculation of mean escape depths (measures of surface sensitivity)[18, 19], for calculation of information depths (measures of sampling depth for a defined fraction of the detected signal)[20], for calculation of emission depth distributions for the signal of interest[18, 20], and for correcting signal intensities for the effects of elastic-electron scattering[17, 21, 22].

NIST ELECTRON INELASTIC-MEAN-FREE-PATH DATABASE (SRD 71)

Version 1.1 of SRD 71 was released in 2000[6]. This database contains electron inelastic mean free paths (IMFPs) calculated from experimental optical data for certain elements and compounds and IMFPs obtained from elastic-peak electron-spectroscopy (EPES) measurements for certain elements[23]. If calculated IMFPs or EPES IMFPs are not available for a material of interest, values can be estimated from the predictive formulae of Tanuma *et al.*[24] or Gries[25]. IMFPs can be displayed graphically or as values for one or more user-selected electron energies. The IMFPs can be presented in different units (Å, nm, or mg/m^2) and in linear, semi-logarithmic, or logarithmic displays. Files containing IMFPs for selected ma-

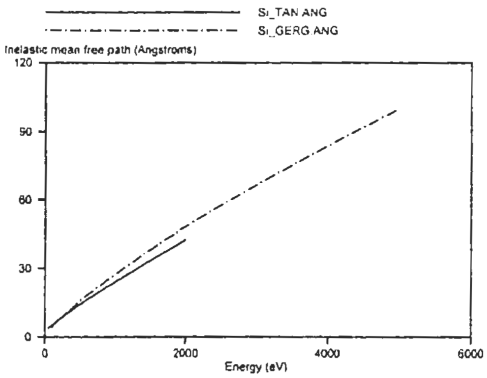

Fig. 3. Comparison of inelastic mean free paths for silicon from the NIST Electron Inelastic-Mean-Free-Path Database. The dot-dashed line shows IMFPs from EPES measurements[30] and the solid line shows IMFPs calculated from optical data[31].

terials can be created, and IMFPs for different materials or from different sources can be graphically compared.

IMFPs are needed in AES and XPS for quantitative analyses (correction of matrix effects)[26, 27], for determination of mean escape depths[18, 19] and information depths[19], for determination of specimen morphology and film thicknesses from analysis of spectral lineshapes[28, 29], and for Monte Carlo simulations of the transport of signal electrons.

As an example, Fig. 3 shows a comparison of IMFPs from SRD 71 for silicon. The dot-dashed line shows IMFPs derived from EPES experiments[30] and the solid line shows IMFPs calculated from experimental optical data[31].

NIST ELECTRON EFFECTIVE-ATTENUATION-LENGTH DATABASE (SRD 82)

Version 1.0 of SRD 82 was released in 2001[5, 6, 15, 16]. This 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 AES and XPS applications. 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. The EAL database incorporates needed transport mean free paths from SRD 64 and inelastic mean free paths from SRD 71. EALs are then calculated using an algorithm based on electron transport theory[32] for measurement conditions specified by the user.

The database supplies "local" EALs (derived from the slope of the emission depth distribution function (DDF) at a specified depth) and "practical" EALs suitable for measurements of overlayer-film thicknesses or depths of thin marker layers[15, 16]. For the latter applications, the database provides a table of practical EALs for a user-specified range of thicknesses or depths. These EALs are plotted as a function of thickness or depth, and an average value shown for a user-selected thickness or depth. An average practical EAL (for thickness measurements) can then be utilized as the "lambda parameter" to obtain overlayer-film thicknesses from simple equations in which the effects of elastic-electron scattering are neglected. A single average practical EAL can generally be employed for electron emission angles up to about 60°. Files with computed EALs can be created and used to prepare plots in which EALs for different conditions or for different materials can be compared. The EAL files and the plots can be printed and stored for use in other applications.

The database also supplies values of other parameters for an infinitely thick material: the mean escape depth [18,19], the correction parameters Q_x and β_{eff} for determination of surface composition by XPS, and the correction parameter Q_A for determination of surface composition by AES[15, 16]. In addition, a user can obtain the DDF for a specified material and measurement configuration, and the

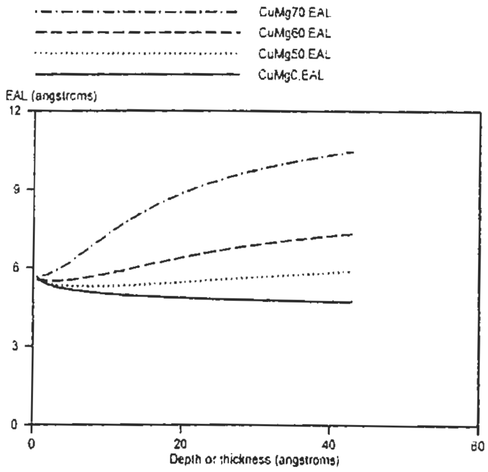

Fig. 4. Plots of practical EALs from the NIST Electron Effective-Attenuation-Length Database for Cu $2p_{3/2}$ photoelectrons excited by Mg Kα x-rays as a function of Cu thickness for an angle ψ between the x-ray source and the analyzer axes of 55° and for emission angles (with respect to the surface normal) of 0° (solid line), 50° (dotted line), 60° (dashed line), and 70° (dot-dashed line).

ratio of this DDF to the DDF found with elastic-electron scattering neglected.

As an example, Fig. 4 shows plots of practical EALs from SRD 82 for Cu $2p_{3/2}$ photoelectrons excited by Mg $K\alpha$ x rays as a function of copper film thickness for four angles of electron emission (with respect to the surface normal). For these photoelectrons, the IMFP was 7.6 Å. We have shown elsewhere that the practical EALs do not vary appreciably with emission angle or with film thickness (in the range of interest for practical AES and XPS) for emission angles between 0° and about 60° [15, 16], and an average value of the EAL can be used for film-thickness measurements. At larger emission angles, however, the practical EALs vary more rapidly with film thickness and emission angle, and it is then necessary to determine the practical EAL by iteration for the particular conditions.

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