Standard Guide for
Background Subtraction Techniques in Auger Electron Spectroscopy and X-Ray Photoelectron Spectroscopy[1]

1. Scope

1.1 The purpose of this guide is to familiarize the analyst with the principal background subtraction techniques presently in use together with the nature of their application to data acquisition and manipulation.

1.2 This guide is intended to apply to background subtraction in electron, X-ray, and ion-excited Auger electron spectroscopy (AES), and X-ray photoelectron spectroscopy (XPS).

1.3 The values stated in SI units are to be regarded as standard. No other units of measurement are included in this standard.

1.4 *This standard does not purport to address all of the safety concerns, if any, associated with its use. It is the responsibility of the user of this standard to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to use.*

2. Referenced Documents

2.1 *ASTM Standards:*[2]
E673 Terminology Relating to Surface Analysis (Withdrawn 2012)[3]

2.2 *ISO Standard:*[4]
ISO 18115–1 Surface chemical analysis—Vocabulary—Part 1: General terms and terms used in spectroscopy

3. Terminology

3.1 *Definitions*—Since Terminology E673 was withdrawn in 2012, for definitions of terms used in this guide, refer to ISO 18115-1.[5]

4. Summary of Guide

4.1 *Relevance to AES and XPS:*

4.1.1 *AES*—The production of Auger electrons by bombardment of surfaces with electron beams is also accompanied by emission of secondary and backscattered electrons. These secondary and backscattered electrons create a background signal. This background signal covers the complete energy spectrum and has a maximum (near 10 eV for true secondaries), and a second maximum for elastically backscattered electrons at the energy of the incident electron beam. An additional source of background is associated with Auger electrons, which are inelastically scattered while traveling through the specimen. Auger electron excitation may also occur by X-ray and ion bombardment of surfaces.

4.1.2 *XPS*—The production of electrons from X-ray excitation of surfaces may be grouped into two categories—photoemission of electrons and the production of Auger electrons from the decay of the resultant core hole states. The source of the background signal observed in the XPS spectrum includes a contribution from inelastic scattering processes, and for non-monochromatic X-ray sources, electrons produced by Bremsstrahlung radiation.

4.2 Various background subtraction techniques have been employed to diminish or remove the influence of these background electrons from the shape and intensity of Auger electron and photoelectron features. Relevance to a particular analytical technique (AES or XPS) will be indicated in the title of the procedure.

4.3 Implementation of any of the various background subtraction techniques that are described in this guide may depend on available instrumentation and software as well as the

method of acquisition of the original signal. These subtraction methods fall into two general categories: (*1*) real-time background subtraction; and (*2*) post-acquisition background subtraction.

5. Significance and Use

5.1 Background subtraction techniques in AES were originally employed as a method of enhancement of the relatively weak Auger signals to distinguish them from the slowly varying background of secondary and backscattered electrons. Interest in obtaining useful information from the Auger peak line shape, concern for greater quantitative accuracy from Auger spectra, and improvements in data gathering techniques, have led to the development of various background subtraction techniques.

5.2 Similarly, the use of background subtraction techniques in XPS has evolved mainly from the interest in the determination of chemical states (from the binding-energy values for component peaks that may often overlap), greater quantitative accuracy from the XPS spectra, and improvements in data acquisition. Post-acquisition background subtraction is normally applied to XPS data.

5.3 The procedures outlined in Section 7 are popular in XPS and AES; less popular procedures and rarely used procedures are described in Sections 8 and 9, respectively. General reviews of background subtraction methods and curve-fitting techniques have been published elsewhere (**1-5**).[6]

5.4 Background subtraction is commonly performed prior to peak fitting, although it can be assessed (fitted) during peak fitting (*active approach* (**6, 7**)). Some commercial data analysis packages require background removal before peak fitting. Nevertheless, a measured spectral region consisting of one or more peaks and background intensities due to inelastic scattering, Bremsstrahlung (for XPS with unmonochromated X-ray sources), and scattered primary electrons (for AES) can often be satisfactorily represented by applying peak functions for each component with parameters for each one determined in a single least-squares fit. The choice of the background to be removed, if required or desired, before or during peak fitting is suggested by the experience of the analysts, the capabilities of the peak fitting software, and the peak complexity as noted above.

6. Apparatus

6.1 Most AES and XPS instruments either already use, or may be modified to use, one or more of the techniques that are described.

6.2 Background subtraction techniques typically require a digital acquisition and digital data handling capability. In earlier years, the attachment of analog instrumentation to existing equipment was usually required.

7. Common Procedures

7.1 The following background subtraction methods are widely employed. It is common for an analyst to choose one

among them depending on the shape of the spectrum. As shown in a Round Robin study, different groups chose different background methods for analyzing the same spectrum (**8**). Although the purpose of this guide is to describe the common procedures employed for background subtraction, 7.3.2 provides a short guide of how to choose one or more background types depending on the shape of the spectrum.

7.2 *Commonly Employed Background Types:*

7.2.1 *Linear Background (AES and XPS)*—In this method, two arbitrarily chosen points in the spectrum are selected and joined by a straight line (**1 and 2**). This straight line is used to approximate the true background and is subtracted from the original spectrum. For Auger spectra, the two points may be chosen either on the high-energy side of the Auger peak to result in an extrapolated linear background or such that the peak is positioned between the two points. For XPS spectra, the two points are generally chosen such that the peak is positioned between the two points. The intensity values at the chosen points may be the values at those energies or the average over a defined number of data points or energy interval. The linear method can be extended to a polynomial version when the peaks are small and riding on top of a more complex (than linear) background (**7**).

7.2.2 *Shirley (or Integral) Background (AES and XPS)*—This method, proposed by Shirley (**9**), employs a mathematical algorithm to approximate the step in the background commonly found at the position of the peak. The algorithm is based on the assumption that the background is proportional to the area of the peak above the background at higher kinetic energy. This implies an iterative procedure, which was described in detail by Proctor and Sherwood (**10**), that should be employed to guarantee self-consistency (**11**). With another variant proposed by Vegh (**12**) and fully discussed by Salvi and Castle (**13**), it is possible to employ a self-consistent Shirley-type background (*SVSC-background*) without the need of an iterative process; it is especially practical for complex spectra (**7**).

7.2.2.1 The original Shirley method was modified by Bishop to include a sloping component to reproduce the decay of the background intensity (**14**). Another modification provides for a background based upon the shape of the loss spectrum from an elastically backscattered electron (**15**), and to include a band gap for insulators (**1**).

7.2.3 *2-Parameter and 3-Parameter Tougaard Backgrounds (XPS)*—This corresponds to a practical version of the approach described in 8.1. Under this method, the λK function, which enters in the algorithm, is taken from a simple universal formula which is approximately valid for some solids. Similar functions have been optimized for particular materials or material classes (**16**). The application of this background might require the acquisition of background data in a 50 to 100 eV range below (in the lower kinetic-energy side) the main peaks. Alternatively, the parameters used in the universal formula may also be permitted to vary in an optimizing algorithm so as to produce an estimate of the background (**1 and 17**). Tougaard has assessed the accuracy of structural parameters and the amount of substance derived from the analysis (**18**). A more approximate form of the Tougaard algorithm (**19**) can be used for automatic processing of XPS spectra (for example, spectra

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