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# Role of consistent terminology in XPS reproducibility

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# Role of consistent terminology in XPS reproducibility

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## ABSTRACT

The use of inconsistent and incorrect terminology in scientific publications contributes to misunderstanding, confusion, and erroneous results in the scientific literature. This issue is of particular importance in x-ray photoelectron spectroscopy (XPS) that is in widespread use for many different purposes by scientists with diverse backgrounds. A set of surface analysis terminology, approved through consensus by international experts, has been developed by International Organization for Standardization Technical Committee TC201 on Surface Chemical Analysis. To encourage wide use, the terminology is accessible at several web sites at no cost. This short overview provides examples to highlight the importance of agreed terminology in eliminating confusion between similar terms. Examples are provided of terms that are commonly misused or confused in the literature. Other examples highlight terminology that provides a common basis for comparing instrument parameters and performance. As science advances, it is important to clarify terminology for describing evolving concepts and developments important to XPS.

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## I. INTRODUCTION

A common understanding of the vocabulary being used is a necessary foundation for communication and advancement of science and technology. Similarly, inconsistent or incorrect use of terminology adds confusion to the literature and inhibits the reproducibility of reported measurements and the testing of conclusions. To address such issues, professional organizations such as the International Union of Pure and Applied Chemistry (IUPAC) and consensus standard organizations including ASTM International and the International Organization for Standardization (ISO) have significant efforts focused on development and maintenance of relevant terminology.

The ISO Committee on Surface Chemical Analysis (TC201), in cooperation with ASTM Committee E42 on Surface Analysis, has developed a set of terminology relevant to surface analysis.<sup>1</sup> A significant part of this terminology is now included in the IUPAC Compendium of Analytical Nomenclature, Glossary of Methods and Terms used in Surface Chemical Analysis.<sup>2</sup> The ISO document currently has two parts: part 1 contains general surface analysis terms and terms related to spectroscopy, while part 2 is focused on scanning probe methods. To facilitate the availability

and use of this terminology, it is web accessible with no fee at several surface analysis oriented websites.<sup>3</sup>

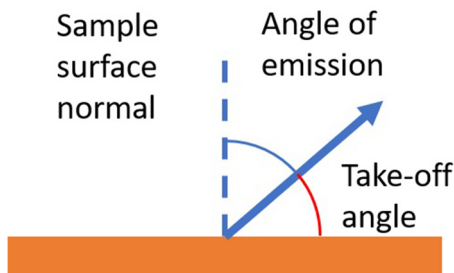
The terminology documents do not attempt to define all terminologies relevant to surface analysis but focus on terminology that has specific relevance or special use in surface analysis. Specific objectives and needs include terminology to (1) clarify the use and definition of terms to minimize multiple or inconsistent usage, (2) provide standard definitions of terminology relevant to instrumentation that enable consistent instrument descriptions and parameter specifications, and (3) assist clarification and descriptions of concepts and the development of new concepts that enable the field to evolve. In Secs. II–IV, examples are provided in each of these areas, highlighting some terminology that has been commonly used inconsistently or incorrectly.

## II. EXAMPLES OF TERMINOLOGY OFTEN MISUSED

### A. Angle of emission and take-off angle

In the early days of x-ray photoelectron spectroscopy (XPS), *take-off angle* and *angle of emission* were both used interchangeably and with different meanings. This led to a good deal of confusion

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**FIG. 1.** Schematic showing the complementary nature of the angle of emission and the take-off angle.

and some contradictory results. The community settled on definitions of these two terms as described in ISO 18115 part 1 as follows:

*angle, take-off* (definition 4.24): angle between the trajectory of a particle as it leaves a surface and the local or average surface plane.

*angle of emission (emission angle)* (definition 4.16): angle between the trajectory of a particle or photon as it leaves a surface, and the local or average surface normal.

These are shown schematically in Fig. 1. Because of the angle sensitivity of XPS measurements and the development of angle resolved XPS, clarity of these definitions was important.

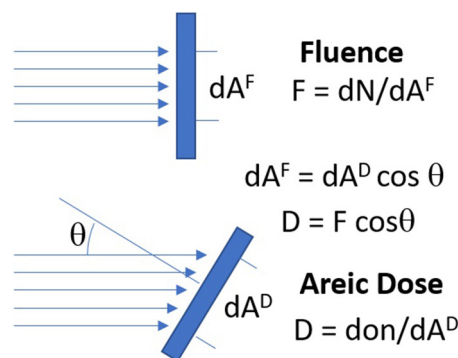
Many of the ISO 18115 definitions have explanatory notes. For take-off angle, note 2 states that the take-off angle complements the angle of emission. Note 3 highlights that in the past, the take-off angle has sometimes been used to erroneously describe the angle of emission.

## B. Fluence and areic dose

Another set of terms often confused and incorrectly reported in publications include fluence and areic dose. Fluence is a term that describes the output of a source of light, electrons or ions, and areic dose is a term related to the sample that is irradiated. This distinction is highly relevant to the calculation of depth in a sputter-depth profile experiment, and a direct quantitative discrepancy arises if fluence is used in the place of areic dose. Because most ion sources are mounted at approximately 45° to the surface, the error associated with confused terminology is approximately 40%. The relevant ISO 18115 definitions are as follows:

*fluence, F* (definition 4.217): (for a parallel beam of particles) the quotient of  $dN$  by  $dA$ , where  $dN$  is the number of particles of a specified type incident on an area  $dA$  at right angles to the direction of the beam:  $F = dN/dA^F$ .

*Areic dose, D* (definition 4.175): the quotient of  $dN$  by  $dA$ , where  $dN$  is the number of energetic particles of a specified type introduced into a solid through a surface area  $dA$ :  $D = dN/dA^D$ .



**FIG. 2.** Schematic highlighting the distinction between fluence and areic dose for parallel stationary beams.

For clarity, we have added the superscripts F and D to differential areas in the above equations. Note the distinction as highlighted in Fig. 2,  $dA^F$  is at right angles to the incoming beam, while this need not be the case for  $dA^D$ . For a stationary (not scanning) parallel beam,  $D = F \cos \theta$ , where  $\theta$  is the angle between the surface normal and the incoming beam. Note 2 for definition 4.217 regarding fluence states that “In some texts, the term *fluence* is used for *areic dose*, which has led to confusion.”

Both fluence and areic dose are associated with the total number of particles that has arrived at a sample. An important related term is flux, the rate at which particles arrive:

*flux ( $\Phi$ )* (definition 4.221): < for a beam of particles > quotient of  $dN$  by  $dt$ , where  $dN$  is the number of particles of a specified type passing in the time interval  $dt$ :  $\Phi = dN/dt$ .

With the definition, a note states that, for a parallel beam with the sample normal parallel to the incoming beam, the fluence rate and flux density are equivalent measures. Here, the fluence rate is the differential of fluence with respect to time, and the flux density is the differential of flux with respect to area on a plane normal to the beam direction. Thus, fluence is the time-dependent integral of flux density but not the time-dependent integral of flux. In depth profiling experiments, where the beam is at an angle to the analyzed surface, the local areic dose rate is required to calculate the areic dose at a given time and position during the experiment. For macroscopically topographic materials, the local angle of the surface and the angle-dependency of the sputtering yield need to be taken into account.

## C. Peak fitting and peak deconvolution

In many circumstances, it is desirable to extract information from XPS spectra that include several peaks, some of which may overlap with others. This is usually accomplished by fitting the peak structure with spectral components. The relevant ISO definitions for this process are *peak fitting* and *peak synthesis*:

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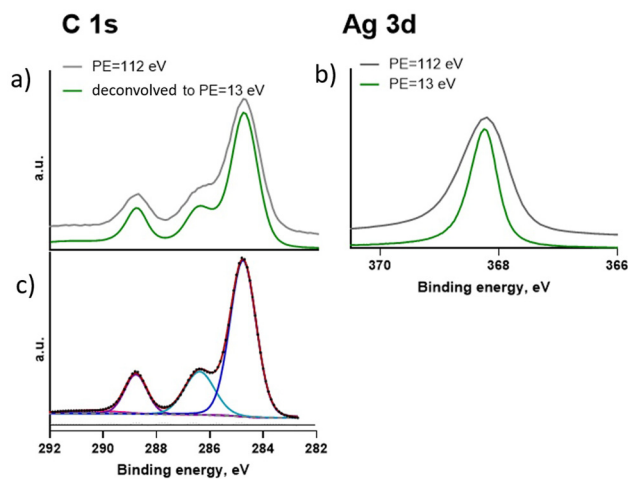
**Peak fitting** (definition 4.328): procedure whereby a spectrum, generated by *peak synthesis*, is adjusted to match a measured spectrum.

**Peak synthesis** (definition 4.329): procedure whereby a synthetic spectrum is generated, using either model or experimental peak shapes, in which the number of peaks, the peak shapes, the peak widths, the peak positions, the peak intensities, and the background shape and intensity are adjusted for peak fitting.

A term frequently applied incorrectly to peak fitting is *deconvolution*, which in surface analysis means using a mathematical procedure to remove line broadening introduced by the finite resolution of the spectrometer.<sup>4</sup> The term *spectrum deconvolution* is defined in an ISO standard (ISO 19830:2015) for reporting requirements for peak fitting in XPS as

*spectrum deconvolution*: mathematical procedures that allow better energy resolution spectra to be calculated from data acquired at a lower resolution. This is achieved by deconvolving the contributions of the spectrometer to the measured spectrum.

Deconvolution was more commonly applied in the early years of XPS when most x-ray sources were achromatic with wider peak widths due to the natural line widths of the x-ray sources. Although it is less needed with monochromatic x-ray sources, there are circumstances when deconvolution is useful. Examples include processing of data when collected at low resolution where



**FIG. 3.** (a) C 1s spectra from PET collected at low (PE 112 eV) energy-resolution and deconvolution of that spectra to higher energy-resolution (roughly equivalent to PE of 13 eV), (b) Ag 3d 5/2 spectra from clean Ag at high and low energy-resolution that were used to construct the deconvolution filter, and (c) fit of the low energy-resolution C 1s spectrum after application of the deconvolution filter. Courtesy of Physical Electronics.

there was a need to collect data rapidly, to observe a time-dependent reaction, to speed up data collection during depth profiles, or to minimize damage to a beam sensitive sample.

An example of deconvolution is shown in Fig. 3. Here, the objective was to demonstrate the application of deconvolution to process low energy-resolution data for possible comparison with data collected at high resolution. The figure shows C 1s spectra from (a) polyethylene terephthalate (PET) collected at low energy-resolution [112 eV pass energy (PE)] and that data deconvolved to higher energy-resolution (roughly equivalent to what could be collected with a PE of 13 eV) and (b) Ag 3d from clean Ag obtained at low and high energy-resolution (112 and 13 eV PE, respectively). The Ag spectra were used to construct a deconvolution filter describing the impact of lower energy resolution on spectra. Application of this filter to the low-resolution C 1s spectrum produced a deconvolved spectrum with increased energy resolution as shown in Fig. 3(a) and with peak fitting as in Fig. 3(c). This approach allows comparison between quickly collected data and higher energy-resolution reference data. For this dataset, the full width half maximum (FWHM) of the C 1s O—C=O peak at 288.8 eV for data collected at PE of 13 eV was 0.82 eV and the FWHM of the peak collected at 112 eV PE was 1.20 eV, and after deconvolution, the FWHM was 0.99 eV.

#### D. Determining chemical states

For many XPS measurements, analysts are interested in learning the chemical nature of elements observed. The link between measurements on the binding energy scale and chemical states is often not as simple and straight forward as many novice users of XPS assume. Terminology in ISO 18115 defines several relevant concepts that appear to be either unknown or ignored in many reports of XPS data in the literature, often leading to misleading or incorrect analysis of the data. Although XPS analysts talk about “binding energy” in relationship to the energy scale by which they measure “peak energies,” it is important to remember the consensus definition of “binding energy” in relationship to an atomic orbital:

*binding energy* (definition 4.82): energy that shall be expended in removing an electron from a given electronic level to the Fermi level of a solid or to the vacuum level of a free atom or molecule.

Elemental identity and chemical state information are usually obtained by determining the energy of a peak, or peaks, in a spectrum:

*peak energy* (definition 4.327): energy value corresponding to the intensity maximum in a direct spectrum or to the intensity minimum for a differential spectrum.

For a variety of reasons, the peak energy on the binding energy scale will be different from the binding energy of the electron in the atom, even if the element is in a well-defined chemical state, the sample is conductive, in contact with the spectrometer and the energy scale of the analyzer properly calibrated. The observed peak energy relates to the energy difference between the initial state of the atom and the final state of the atom:

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*initial state* (definition 4.249): ground state of an atom prior to photoelectron emission.

*final state* (definition 4.215): state of an atom resulting after a particular Auger, X-ray, or photoemission process.

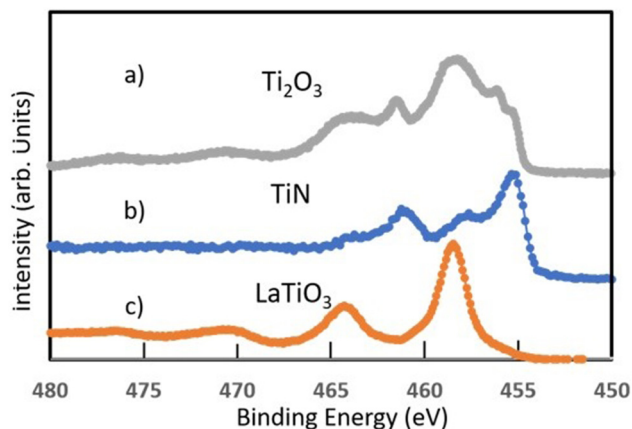
Although there is only one initial state, there may be many accessible final states. Several processes that occur in the final state can influence the measured peak energy including multiplet splitting (definition 4.313), shakeup (definition 4.423), and shakeoff (definition 4.422) processes. These often manifest as broadened peaks or multiple peaks.

In some cases, such as C1s spectra of organic materials, the initial state effects are more important than the final state effects, and the change in peak energy may be related to the local charge on the emitting atom. The shift in peak energy between different chemical states in such cases is very useful and is called the chemical shift:

*chemical shift* (definition 4.105): change in peak energy (4.327) arising from a change in the chemical environment of the atom.

In other cases, the chemical shift will not be intuitive and may even be difficult to define if there is significant structure due to final state effects.

Ignoring the basic physical and chemical processes has led to a significant number of errors in the XPS analysis of data in the literature.<sup>5</sup> One common error is incorrect identification of peaks arising from spin-orbit coupling, multiplet splitting, and shakeup processes as indications of multiple chemical states. Inexperienced analysts may misinterpret small peaks or peak shifts due to final state processes generally and shakeup or shakeoff effects' features specifically as new or additional chemical states. To highlight the potential impacts of these effects, examples of different peak shapes for Ti 2p are shown in Fig. 4. Although the formal oxidation state of Ti in



**FIG. 4.** XPS Ti 2p spectra from three materials that contain Ti formally with +3 oxidation state: (a)  $\text{Ti}_2\text{O}_3$ , (b) TiN, and (c)  $\text{LaTiO}_3$ . Final state effects contribute to the variations in the peak structure also demonstrating that the binding energy of the peak is not a simple indicator of the chemical state.

$\text{Ti}_2\text{O}_3$  (1012),<sup>6</sup> TiN,<sup>7</sup> and epitaxial  $\text{LaTiO}_3$  (001)<sup>8</sup> is +3, the spectra have significantly different peak shapes due to final state effects.

### III. TERMINOLOGY RELATED TO INSTRUMENT PERFORMANCE

Many parameters or specifications for an XPS instrument are easily defined such as type of x-rays available, allowed sample size, analyzer type, and the count rate for Ag for conditions for which the FWHM of the Ag 3d<sub>5/2</sub> has some specified value. In some cases, instrument performance is determined by a measurement in relation to some defined conditions. Figures of importance for some applications and instrument comparison are the *energy resolution* of the electron spectrometer for specific conditions (e.g., pass energy, aperture size) and the *lateral resolution* available during an XPS measurement and the area of a sample being analyzed (*analysis area*). ISO 18115 has relevant definitions for each of these. An important feature of each of these parameters is that the values will depend both upon the instrument operation parameters (e.g., x-ray source conditions or analyzer settings) and the selection of how they are measured, as discussed below. One such parameter is lateral resolution:

*Lateral resolution* (def. 4.385) distance, measured either in the plane of the sample surface (4.458) or in a plane at right angles to the axis of the image-forming optics, over which changes in composition can be separately established with confidence.

This parameter is a measure of the ability to separate or distinguish XPS spectral information from different regions of a sample. Methods and challenges to reproducible small-spot resolution are discussed in a guide by Unger *et al.*<sup>9</sup> One measure of lateral resolution involves measurements across a “knife edge” or other sharply defined regions in a test sample. The resolution (or beam size) is typically identified/defined by the distance between symmetric intensity points (12% and 88%, 16% and 84%, or 20% and 80%). Awareness of the actual parameters used to determine lateral resolution can be important in comparing instruments or data.

Lateral resolution is sometimes assumed to simply relate to the area that would be analyzed but, just as there are differences based on the percentages of signals observed in the measurements of lateral resolution, there are similar differences in how an area of analysis might be determined.

*Analysis area* (def 4.8) two-dimensional region of a sample surface measured in the plane of that surface from which the entire analytical signal or a specified percentage of that signal is detected.

The area analyzed during an XPS measurement can be influenced by both the lens of the analyzer and properties of the x-ray beam. Although the “size” of the beam or analysis area is often identified or described by a measurement of the *lateral resolution* for the measurement conditions being applied, the actual area of analysis may be better represented by measurements of the signal intensity of an element outside a circular region of known diameter.<sup>9,10</sup> Plots of the signal from inside or outside a circular region of known size

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on a reference sample can be compared to a lateral resolution measurement.

Results from a set of measurements involving circular features containing Cr surrounded by indium tin oxide are shown in Fig. 5. These measurements involved an instrument for which the x-ray beam size determined the resolution and involved two types of measurements: (1) one beam size ( $d_b$ ), defined by a 16%–84% measurement of lateral resolution, was used during measurements from a variety of circular spots of different diameters ( $D$ ) and (2) different beam sizes ( $d_b$ ) were applied to measurements of signals from a single circular spot of diameter  $D$ . The approach and details are described in Ref. 10. When plotted as a ratio of signal from inside the spot versus outside the spot as a function of  $D/d_b$ , the results from both measurement approaches produced similar results. An important message from the plot is that when the diameter of the circular feature was twice the measured beam resolution size, more than 40% of the signal came from outside the feature. The dashed curve in Fig. 5 is the behavior expected if the acceptance area relative to feature size had a Gaussian profile and was ideally centered. The two curves that approximately model the data points in Fig. 5 have beam intensities that fall off as  $1/r^3$ , where  $r$  is the distance from the center of the beam. These specific results are for one instrument with a specific operating condition, but the results serve as an illustration of the danger in confusing lateral resolution with analysis area and in assuming an idealized shape for the lateral response of the instrument. Analysis area and lateral resolution may be quantified in a similar manner, using similar units, but they describe different things. Standard reference samples are being

created to facilitate determination of analysis area relevant to analytical needs.<sup>11</sup>

Resolution terminology is sometimes framed within the context, assumption, or approximation of Gaussian shapes or distributions. For example, if the lateral resolution of an instrument had Gaussian and symmetrical behavior, the 16%–84% size determination would correspond to two-sigma width. However, as suggested in Fig. 5, the analysis area does not always have Gaussian behavior. In this case, it appears that the 16%–84% determination of diameter of the analysis area does not adequately reflect the “tails” in the detected signal distribution.

Concepts of resolution are important in many of the definitions included in ISO 18115, and the historical conventions and definitions of resolution do not necessarily adequately meet the current needs or adequately address some of the relevant concepts and needs as instrumentation advances. Terminology must adjust and expand to represent current needs and understandings. Consequently, terminology and concepts associated with resolution are being examined and revised as appropriate for the next version of ISO 18115 part 1 to accommodate the variety of analysis needs. A note proposed for a new definition of resolution indicates that “In practice, many different resolution criteria are used. The choice will depend on the measurand, the circumstances and the required use of the measure.”

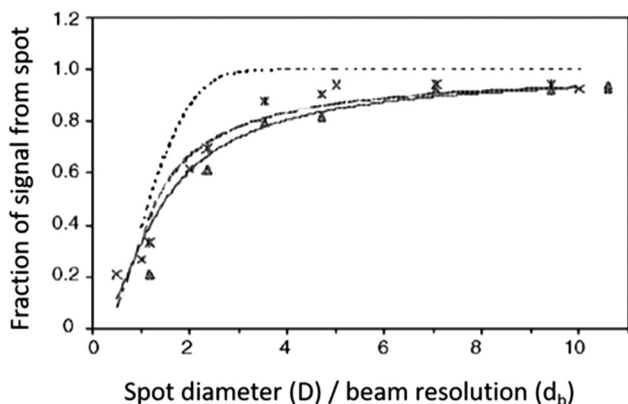
#### IV. ADJUSTING TO NEW CONCEPTS—TERMINOLOGY RELATED TO XPS ANALYSIS DEPTHS

In the *Practical Guide for Inelastic Mean Free Paths (IMFP), Effective Attenuation Lengths (EAL), Mean Escape Depths (MED), and Information Depths (ID) in X-ray Photoelectron Spectroscopy*,<sup>12</sup> Powell observed that:

Many experiments were performed in the 1960s and 1970s to determine the surface sensitivity of AES and XPS. Thin films of a known thickness were deposited on substrates of another material, and measurements were made of the intensities of Auger-electron peaks or photoelectron peaks from the substrate or overlayer materials as a function of overlayer thickness. The substrate intensities were often found to decrease exponentially with overlayer thickness, and the overlayer intensities were similarly found to increase exponentially with thickness (...). The resulting exponential parameters were then regarded as useful measures of surface sensitivity and were termed “inelastic mean free paths,” “attenuation lengths,” or “escape depths.” These terms were then thought to be synonymous and were used interchangeably.

The importance of elastic scattering in addition to inelastic scattering has since been recognized. Consequently, terminology needed to be revised, and each of the above terms now has a separate definition that is included in ISO 18115 part 1.<sup>12</sup>

Based on current understandings, the IMFP is an energy-dependent material parameter. However, EALs, IDs, and MEDs depend on both the IMFPs and instrument configuration and, in particular, the specific application for the EAL. In the early measurements of what we now call EALs, it was assumed that only inelastic scattering occurred, i.e., the electrons lost energy when



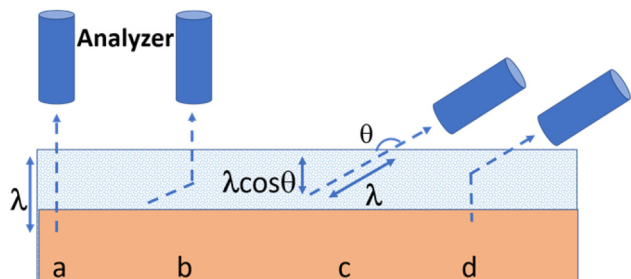
**FIG. 5.** Fraction of signal intensity collected from inside a circular region “spot” as a function of the ratio of the spot diameter ( $D$ ) to the beam diameter ( $d_b$ ) determined by the 16%–84% edge resolution method. Two types of data sequences are shown in the figure: (1) two series of data ( $\Delta$ ,  $\star$ ) collected for which the beam diameter was held constant and the spot size varied and (2) a series ( $\times$ ) for which the spot size remained constant and the beam diameter varied. The dashed curve is behavior expected for the acceptance area or beam size with a Gaussian profile. The other curves are for models of acceptance with “tails” that fall off as  $1/r^3$ , where  $r$  is the radius from the center of the measured spot. Details of the measurements and models can be found in Ref. 10. From Baer and Engelhard, *Surf. Interface Anal.* **29**, 766, 2000. Copyright 2000, Wiley and Sons.

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scattered and otherwise travelled in a straight line and that the IMFP was identical to the EAL. It is now known that elastic scattering is a significant effect, and a straight-line path cannot be assumed. As a result, the EAL that is used for overlayer thickness measurements using XPS, as described by Powell,<sup>12</sup> can differ from the IMFP by up to 40%.

The schematic drawing in Fig. 6 shows how elastic scattering can impact an XPS measurement. For presentation simplicity, we consider that an electron can travel in a straight line one IMFP before inelastic scattering and look at consequences of elastic scattering on angle dependent XPS measurements. If we are detecting electrons of specific energy and analyzing electrons with a 0° angle of emission, the analysis depth would be equal to the IMFP ( $\lambda$ ) [Fig. 6(a)]. For normal emission, electrons within one  $\lambda$  would be detected by the analyzer. The presence of elastic scattering [Fig. 6(b)], which changes direction but not energy, increases the number of electrons within  $\lambda$  that would be detected at normal emission. More electrons arising from a shallower depth not initially directed toward the analyzer can be directed into the analyzer by elastic scattering. Conversely, electrons from deeper layers (nearly equal in depth  $\lambda$ ) would tend to be directed away from the analyzer by elastic scattering. Thus, in this case, the EAL is smaller than the IMFP. When looking at a 60° angle of emission, the effective straight-line depth decreased to  $\lambda \cos(60^\circ)$  [Fig. 6(c)]. However, with elastic scattering, an electron arising from depths greater than  $\lambda \cos(60^\circ)$  may be scattered into the detector without energy loss [Fig. 6(d)]. Calculations indicate that effects of elastic scattering tend to make EALs less than IMFPs for emission angles between 0° and 55° and EALs greater than IMFPs for emission angles greater than 60°.<sup>13</sup>

This example schematically shows the reason that the initial single concept of IMFP expanded to consideration of the EAL for



**FIG. 6.** Schematic drawing indicating the effects of elastic scattering on analysis depths and angle resolved signals. Note that elastic scattering is ignored in (a) and (c) and electrons are assumed to travel in a straight line before emission from the sample and being detected. Elastic scattering (no energy loss) is indicated in (b) and (d). (a) For normal emission, electrons within one  $\lambda$  would be detected by the analyzer. (b) Elastic scattering effectively increases the fraction of electrons within depth  $\lambda$  that would be detected at normal emission. (c) For angular emission and no elastic scattering, the depth into the sample changes with the cosine of the angle of emission. (d) With elastic scattering, electrons originating at depths deeper than  $\lambda \cos\theta$  may be directed into the analyzer. Elastic scattering tends to make EALs less than IMFPs for emission angles between 0° and 55° and EALs greater than IMFPs for emission angles greater than 60°.

describing measured photoelectron intensities and required refinement of the relevant terminology. Along with needs for more sophisticated terminology related to resolution, the advancement of electron path length concepts provides a second example of why terminology needs to change and evolve with time.

## V. SUMMARY AND CONCLUSIONS

Consistent and correct use of terminology is an important component of scientific advancement and highly relevant to reliable and reproducible data reports in the literature. Because of this importance, the ISO Technical Committee 201 on Surface Chemical Analysis has made the terminology in ISO 18115 available at websites<sup>3</sup> hosted by the following organizations: American Vacuum Society (AVS), UK National Physical Laboratory (NPL), Environmental Molecular Sciences Laboratory (EMSL) at Pacific Northwest National Laboratory (PNNL) [USA], Surface Analysis Society of Japan (SASJ) [Japan], National Institute of Advanced Industrial Science and Technology (AIST) [Japan], Physikalisch-Technische Bundesanstalt (PTB) [Germany], Bundesanstalt für Materialforschung und prüfung (BAM) [Germany], and Spanish Vacuum Society (ASEVA).

Clear terminology is essential for scientific communication to ensure consistency, concept clarity, and accuracy. As concepts evolve, terminology needs to change to meet current understandings and needs. The terminology discussed in this paper is based primarily on ISO 18115 that has been developed over the past 40 years with contributions from experts around the world through the consensus standards processes of ASTM and ISO. Definitions are not static and frequently need clarification. The authors welcome suggestions for needed changes, clarifications, or additional terms. Such suggestions can be made to the authors, TC201 participants in National Standards Organizations, or to the current chair or secretary of ISO TC201.

## ACKNOWLEDGMENTS

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- <sup>3</sup>Websites hosting ISO 18115 terminology: American Vacuum Society (AVS): <http://www.avs.org/Technical-Library/Technical-Resources>; UK National Physical Laboratory: <https://www.npl.co.uk/surface-technology/standardisation-traceability>; Environmental Molecular Sciences Laboratory: <https://www.emsl.pnnl.gov/emslweb/vocabulary-definitions>; Surface Analysis Society of Japan (SASJ): <http://www.sasj.jp/iso/ISO18115.html>; National Institute of Advanced Industrial Science and Technology: [http://www.aist.go.jp/aist\\_e/dept/iso.html](http://www.aist.go.jp/aist_e/dept/iso.html); PTB Germany:

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