**Designation: E1636 – 10**

# Standard Practice for
# Analytically Describing Depth-Profile and Linescan-Profile Data by an Extended Logistic Function[1]

This standard is issued under the fixed designation E1636; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last reapproval. A superscript epsilon (ε) indicates an editorial change since the last revision or reapproval.

## 1. Scope

1.1 This practice describes a systematic method for analyzing depth-profile and linescan data and for accurately characterizing the shape of an interface region or topographic feature. The profile data are described with an appropriate analytic function, and the parameters of this function define the position, width, and any asymmetry of the interface or feature. The use of this practice is recommended in order that the shapes of composition profiles of interfaces or of linescans of topographic features acquired with different instruments or techniques can be unambiguously compared and interpreted.

1.2 This practice is intended to be used for two purposes. First, it can be used to describe the shape of depth-profiles obtained at an interface between two dissimilar materials that might be measured by common surface-analysis techniques such as Auger electron spectroscopy, secondary-ion mass spectrometry, and X-ray photoelectron spectroscopy. Second, it can be used to describe the shape of linescans across a detectable topographic feature such as a step or a feature on a surface that might be measured by a surface-analysis technique, scanning electron microscopy, or scanning probe microscopy. The practice is particularly valuable for determining the position and width of an interface in a depth profile or of a feature on a surface and in assessments of the width as an indication of the sharpness of the interface or feature (a characteristic of the material system being measured) or of the achieved depth resolution of the profile or the lateral resolution of the linescan (a characteristic of the particular analytical technique and instrumentation).

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]
E1127 Guide for Depth Profiling in Auger Electron Spectroscopy
E1162 Practice for Reporting Sputter Depth Profile Data in Secondary Ion Mass Spectrometry (SIMS)
E1438 Guide for Measuring Widths of Interfaces in Sputter Depth Profiling Using SIMS

2.2 *ISO Standards:*[4]

ISO 18115 Surface Chemical Snalysis – Vocabulary, 2001; Amd. 1:2006, Amd. 2:2007
ISO 18516 Surface Chemical Analysis – Auger Electron Spectroscopy and X-Ray Photoelectron Spectroscopy – Determination of Lateral Resolution, 2006

## 3. Terminology

3.1 *Definitions*—For definitions of terms used in this practice, see Terminology E673 and ISO 18115.

3.2 *Definitions of Terms Specific to This Standard:*

3.2.1 Throughout this practice, three regions of a *sigmoidal profile* will be referred to as the *pre-interface*, *interface*, and *post-interface* regions. These terms are not dependent on whether a particular interface or feature profile is a growth or a decay curve. The terms *pre-* and *post-* are taken in the sense of increasing values of the independent variable *X*, the depth (for a depth profile) or the lateral position on the surface (for a linescan).

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[1] This practice is under the jurisdiction of ASTM Committee E42 on Surface Analysis and is the direct responsibility of Subcommittee E42.08 on Ion Beam Sputtering.

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[2] For referenced ASTM standards, visit the ASTM website, www.astm.org, or contact ASTM Customer Service at service@astm.org. For *Annual Book of ASTM Standards* volume information, refer to the standard's Document Summary page on the ASTM website.

[3] The last approved version of this historical standard is referenced on www.astm.org.

[4] Available from International Organization for Standardization (ISO), 1, ch. de la Voie-Creuse, Case postale 56, CH-1211, Geneva 20, Switzerland, http://www.iso.ch.

## 4. Summary of Practice

4.1 Depth-profile data for an interface (that is, signal intensity or composition versus depth) or linescan data (that is, signal intensity or composition versus position on a surface) are fitted to an analytic function, an extended form of the logistic function, in order to describe the shape of such profiles.[5,6] Least-squares fitting techniques are employed to determine the values of the parameters of this extended logistic function that characterize the shape of the interface. The interface width, depth or position, and asymmetry are determined from these parameters.

## 5. Significance and Use

5.1 Information on interface composition is frequently obtained by measuring surface composition while the specimen material is gradually removed by ion bombardment (see Guide E1127 and Practice E1162). In this way, interfaces are revealed and characterized by the measurement of composition versus depth to obtain a sputter-depth profile. The shape of such interface profiles contains information about the physical and chemical properties of the interface region. In order to accurately and unambiguously describe this interface region and to determine its width (see Guide E1438), it is helpful to define the shape of the entire interface profile with a single analytic function.

5.2 Interfaces in depth profiles from one semi-infinite medium to another generally have a sigmoidal shape characteristic of the cumulative logistic distribution. Use of such a logistic function is physically appropriate and is superior to other functions (for example, polynomials) that have heretofore been used for interface-profile analysis in that it contains the minimum number of parameters for describing interface shapes.

5.3 Measurements of variations in signal intensity or surface composition as a function of position on a surface give information on the shape of a step or topographic feature on a surface or on the sharpness of an interface at a phase boundary. The shapes of steps or other features on a surface can give information on the lateral resolution of a surface-analysis technique if the sample being measured has sufficiently sharp edges (see ISO 18516). Similarly, the shapes of compositional variations across a surface can give information on the physical and chemical properties of the interface region (for example, the extent of mixing or diffusion across the interface). It is convenient in these applications to describe the measured linescan profile with an appropriate analytic function.

5.4 Although the logistic distribution is not the only function that could be used to describe measured linescans, it is physically plausible and it has the minimum number of parameters for describing such linescans.

5.5 Many attempts have been made to characterize interface profiles with general functions (such as polynomials or error functions) but these have suffered from instabilities and an inability to handle poorly structured data. Choice of the logistic function along with a specifically written least-squares procedure (described in Appendix X1) can provide statistically evaluated parameters that describe the width, asymmetry, and depth of interface profiles or linescans in a reproducible and unambiguous way.

## 6. Description of the Analysis

6.1 *Logistic Function Data Analysis*—The logistic function was first named and applied to population growth in the 20th century by Verhulst.[7] In its simplest form, this function may be written as:

$$Y = \frac{1}{1+e^{-x}} \tag{1}$$

in which $Y$ progresses from 0 to 1 as $X$ varies from $-\infty$ to $+\infty$. The differential equation generating this function is:

$$dY/dX = Y(1-Y) \tag{2}$$

and in this form describes a situation where a measurable quantity $Y$ grows in proportion to $Y$ and in proportion to finite resources required by $Y$. Appropriate to an interface, the propensity for change in the fractional composition of a species at a particular boundary is proportional to the concentration of that species at the boundary and the concentration of the other species at the adjacent boundary. The logistic function as a distribution function and growth curve has been extensively reviewed by Johnson and Kotz.[8] Interface or linescan profile data are usefully fitted to an extended form of the logistic function:

$$\begin{aligned} Y = {} & [A + A_s(X - X_0)]/(1+e^{z}) \\ & + [B + B_s(X - X_0)]/(1+e^{-z}) \end{aligned} \tag{3}$$

where:

$$z = (X - X_0)/D \tag{4}$$

and:

$$D = 2D_0/[1+e^{Q(X-X_0)}] \tag{5}$$

6.1.1 $Y$ is a measured signal (for example, from a surface-analysis instrument, a scanning electron microscope, or a scanning probe microscope) or a measure of the elemental surface concentration of one of the components and $X$, the independent variable, is a measure of the sputtered depth, usually expressed as a sputtering time, or lateral position on the surface. Pre-interface and post-interface signals or surface concentrations are described by the parameters $A$ and $B$, respectively, and the parameters $A_s$ and $B_s$ are introduced to account for any time-dependent instrumental effects or otherwise to better describe the shape of the measured profile. $X_0$ is the midpoint of the interface region (depth or time for a profile or of position for a linescan). The scaling factor $D_0$ is a

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[5] Kirchhoff, W. H., Chambers, G. P., and Fine, J., "An Analytical Expression for Describing Auger Sputter Depth Profile Shapes of Interfaces," *Journal of Vacuum Science and Technology A*, Vol 4, 1986, p. 1666.

[6] Wight, S. A. and Powell, C. J., "Evaluation of the Shapes of Auger- and Secondary-Electron Line Scans across Interfaces with the Logistic Function," *Journal of Vacuum Science and Technology A*, Vol 24, 2006, p. 1024.

[7] Verhulst, P. F., *Acad. Brux*, Vol 18 , 1845, p. 1.

[8] Johnson, N. L., and Kotz, S., *Distributions in Statistics: Continuous Univariate Distributions*, Chapter 22, Houghton Mifflin Co., Boston, 1970.

characteristic depth for sputtering through the interface region of a depth profile or a characteristic width for a linescan; $Q$, an asymmetry parameter, is a measure of the difference in curvature in the pre- and post-interface ends of the interface region. Conventional measures of the interface width can be determined from $D_0$ and $Q$. Fig. 1 shows examples of profile shapes from Eq 3-5 for illustrative values of $D_0$ and $Q$.[5]

6.2 Fitting of interface-profile data to the above function, Eq 3, can be accomplished by using least-squares techniques. Because these equations are non-linear functions of the three transition-region parameters, $X_0$, $D_0$, and $Q$, the least-squares fit requires an iterative solution. Consequently, $Y$, as expressed by Eq 3, can be expanded in a Taylor series about the current values of the parameters and the Taylor series terminated after the first (that is, linear) term for each parameter. $Y(\text{obs}) - Y(\text{calc})$ is fitted to this linear expression and the least-squares routine returns the corrections to the parameters. The parameters are updated and the procedure is repeated until the corrections to the parameters are deemed to be insignificant compared to their standard deviations. Values for interface width, depth, and asymmetry can be calculated from the parameters of the fitted logistic function. The iterative solution also requires a robust means for making initial estimates of the parameter values.

6.3 Implementation of this procedure can be readily accomplished by making use of a specialized computer algorithm and supporting software (logistic function profile fit (LFPF)) developed specifically for this application and described in Appendix X1.

6.3.1 The fitting can also be done in Excel, using the solver option to determine the variables $A$, $B$, $A_s$, $B_s$, $X_0$, $D_0$, and $Q$. Write the definition of the logistic function (Eq 3-5) in Excel and calculate its values as a function of $X$. If the exponential function $e^z$ produces overflow when $z > 709$, this problem can easily be circumvented by writing EXP (min ($z$, 709)) instead of EXP($z$).

6.3.2 The fitting can also be done with any suitable nonlinear least-squares software that is available.

## 7. Interpretation of Results

7.1 The seven parameters necessary to characterize the interface-profile shape are determined by a least-squares fit of the interface data to the extended logistic function. These parameters are related to the three distinct regions of the interface profile. Two parameters, an intercept $A$ and a slope $A_s$ are necessary to define the pre-interface asymptote while two more, $B$ and $B_s$, define the post-interface asymptote. For the analysis of many interface profiles, it may be satisfactory to assume that both of the slope parameters, $A_s$ and $B_s$, are zero. Two more parameters, $D_0$ and $X_0$, define the slope and position of the transition region. In addition, an asymmetry parameter $Q$ that causes the width parameter to vary logistically from 0 to $2D_0$, is introduced as a measure of the difference in curvature in the pre- and post-transition ends of the transition region. If $Q < 0$, the pre-transition region has the greatest (sharpest) curvature. If $Q > 0$, the post-transition region has the greatest curvature. If $Q = 0$, $D = D_0$ and the transition profile is symmetric. The parameter $Q$ has the dimensions of $1/x$ whereas

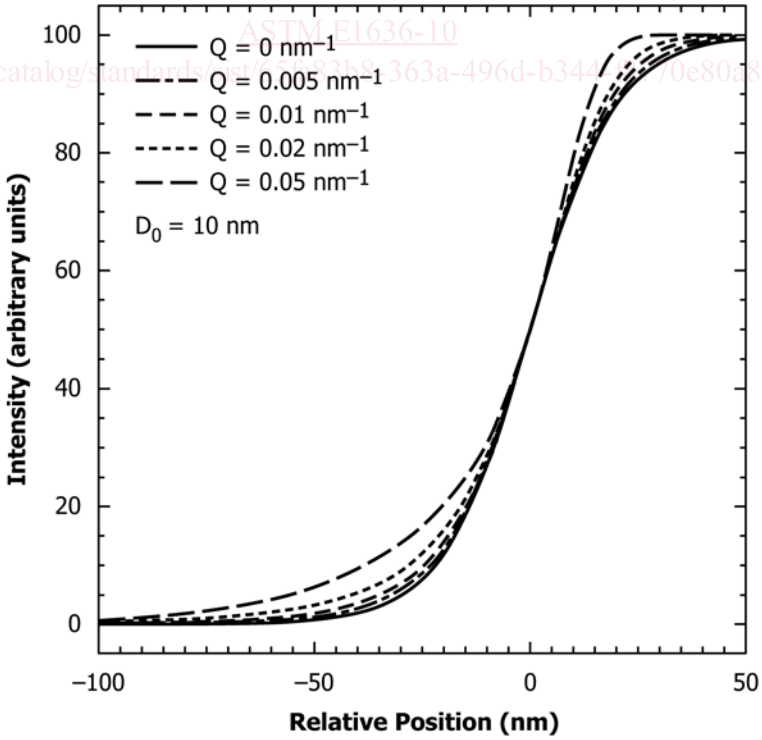
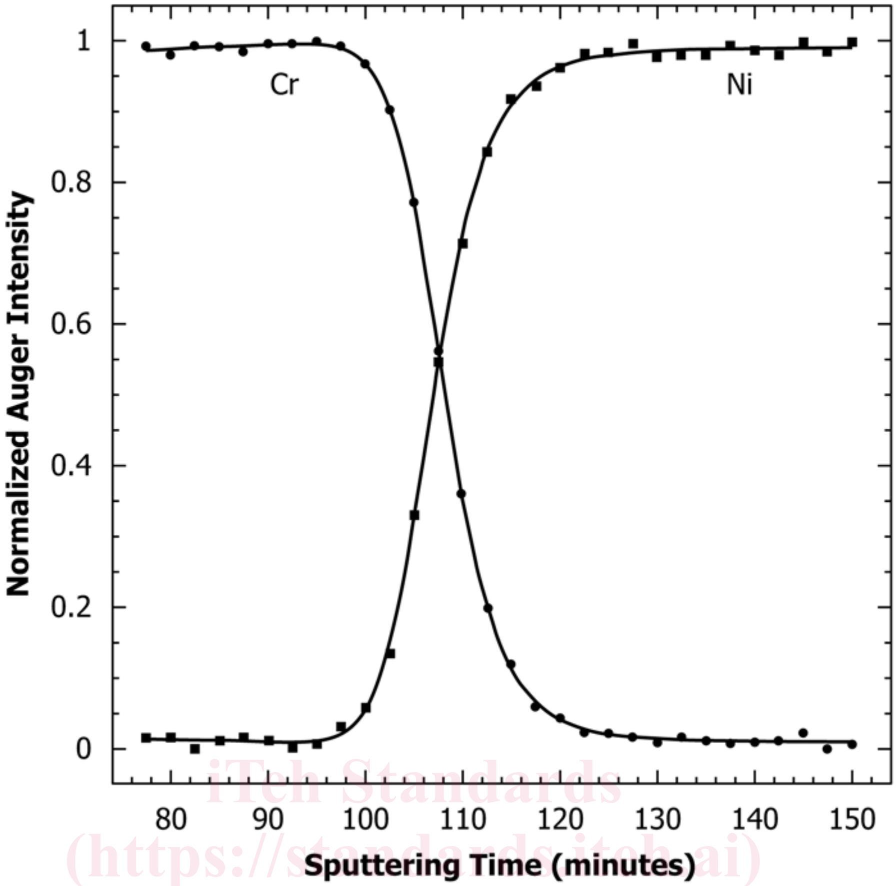


**FIG. 1 Plot of Eq 3-5 Showing Relative Intensity as a Function of Relative Position $X$ with $A = A_s = B_s = X_0 = 0$, $B = 100$, $D_0 = 10$ nm, and the Indicated Values of $Q$ (from the paper referenced in Footnote 5)**



NOTE 1—The solid lines are the profiles calculated from the least-squares parameters shown in Table 2.

**FIG. 2 Results of the Least-Squares Fit of the Simulated Cr and Ni Auger Intensities (Symbols) in Table 1 to the Extended Logistic Function of Eq 3**

$D_0$ has the dimensions of $X$. The product $QD_0$ is dimensionless and is a measure of the asymmetry of the profile independent of its width. If the absolute magnitude of $QD_0$ is less than 0.1, the asymmetry in the transition profile should be barely discernible. Fig. 1 shows illustrative plots of the logistic function (Eq 3-5) for values of $QD_0$ 0, 0.05, 0.1, 0.2, and 0.5.

7.2 The final results should include the calculated values of $Y$ and associated statistics, the values of the determined parameters and their uncertainties, and statistics related to the overall quality of the least-squares fit.

7.3 The width of the interface region, $I_f$, is the depth (time) or distance required for the decay or growth curve to progress from a fraction $f$ of completion to $(1-f)$ of completion. For the case where $Q = 0$, $I_f$ is proportional to $D_0$ and is given by the simple formula:

$$I_f = 2D_0 \ln[(1-f)/f] \qquad (6)$$

so that, for example, the traditional 16 % to 84 % interface width is 3.32 $D_0$. Similarly, the interface widths determined from the 10 % to 90 %, 12 % to 88 %, 20 % to 80 %, and 25 % to 75 % intensity changes are $4.39D_0$, $3.99D_0$, $2.77D_0$, and $2.20D_0$, respectively.

7.4 Introduction of the asymmetry parameter $Q$ into the extended logistic function makes the calculation of the 16 % to 84 % points of the interface more complicated. In particular, for fractions $f$ and $(1-f)$ of completion of the interface transition:

$$X_f = X_0 + 2\,D_0 \ln[f/(1-f)]/[1+e^{Q(X_f-X_0)}] \qquad (7)$$

and:

$$X_{(1-f)} = X_0 + 2\,D_0 \ln[(1-f)/f]/[1+e^{Q(X_{1-f}-X_0)}] \qquad (8)$$

$X_f$ and $X_{(1-f)}$ (which appear on both sides of Eq 7 and Eq 8) can be evaluated most readily by Newton's method of successive approximations.

## 8. Reporting of Results

8.1 Interface profile shapes can be accurately characterized by the extended logistic function and its parameters. Results of such interface analysis should report these parameters ($X_0$, $D_0$, and $Q$) together with their uncertainties, the standard deviation of the fit, and an interface width obtained from $D_0$ and $Q$ that is based on an accepted definition (for example, 16 % to 84 % signal or concentration change; see also ISO 18516).

8.2 The sputtered depth, $X$, is often difficult to determine experimentally so that depth profile data are normally acquired with time as the independent variable. This sputtered time can be referenced with respect to a removal time obtained with a