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).

[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.

Current edition approved Jan. 1, 2010. Published March 2010. Originally approved in 1999. Last previous version approved in 2004 as E1636 – 04. DOI: 10.1520/E1636-10.

[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:

$$Y = [A + A_s(X - X_0)]/(1+e^{z}) \tag{3}$$

$$+[B + B_s(X - X_0)]/(1+e^{-z})$$

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

[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(obs) – Y(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

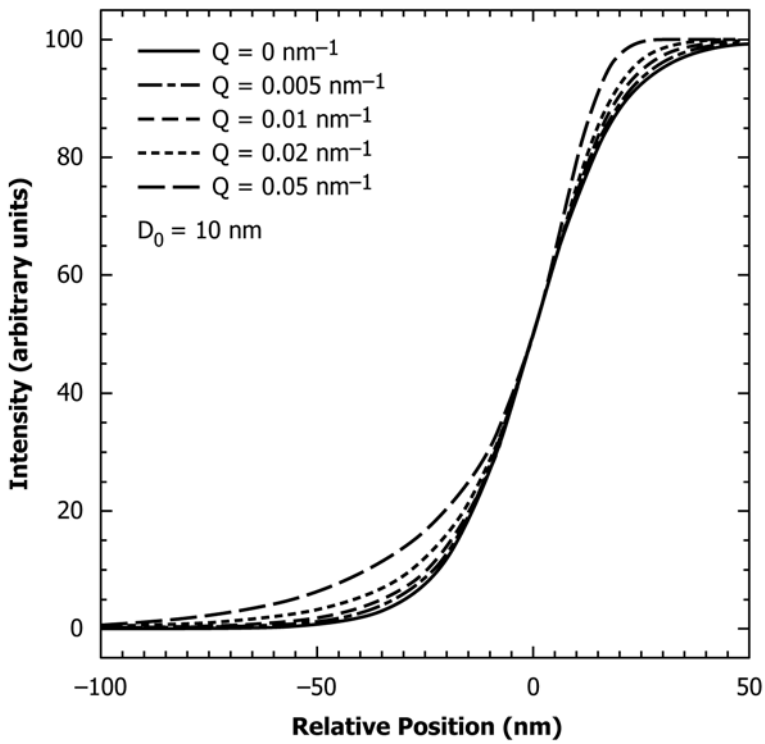
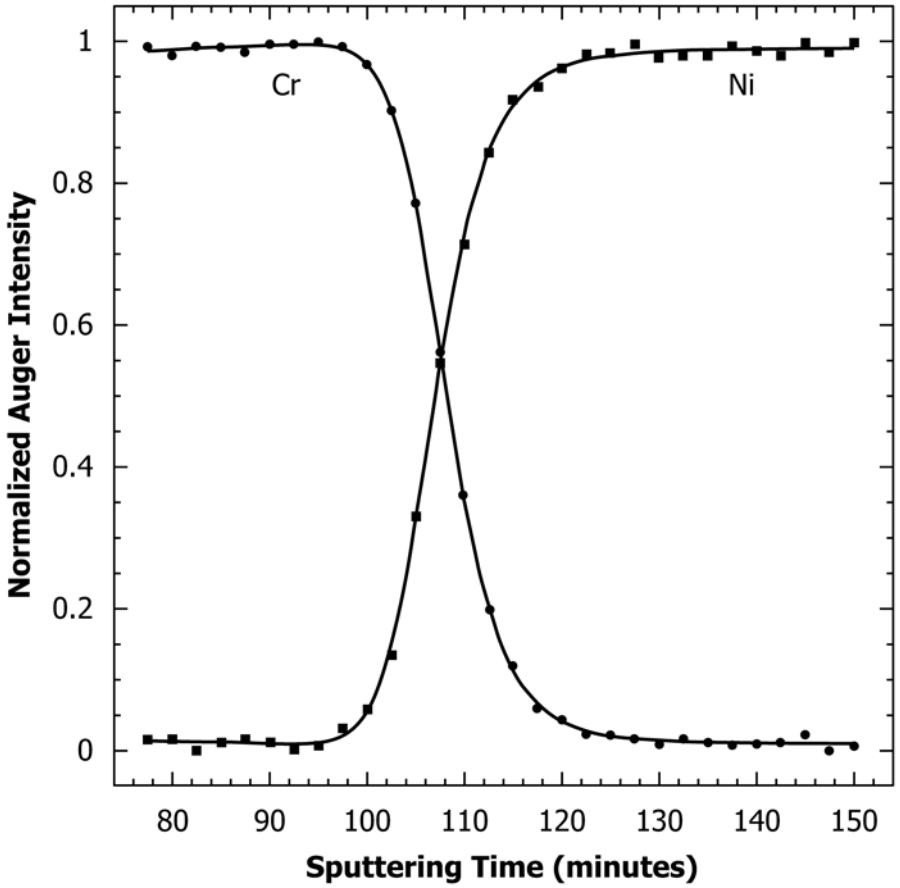


FIG. 1 Plot of Eq 3-5 Showing Relative Intensity as a Function of Relative Position X with $A = A_s = B_s = X_0 = 0$, $B = 100$, $D_0 = 10$ nm, and the Indicated Values of Q (from the paper referenced in Footnote 5)



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:

$$I_f = 2D_0\, 1n\,[(1 - f)/f] \tag{6}$$

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:

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

and:

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

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

TABLE 1 Simulated Auger Intensities for a Cr/Ni Interface to be Used for Comparison of Computational Approaches

NOTE 1—The Cr and Ni intensities have been normalized to range between 0 and 1.

Time (min)	Cr Intensity	Ni Intensity
77.5	0.9932	0.0155
80.0	0.9796	0.0158
82.5	0.9933	0.0000
85.0	0.9923	0.0113
57.5	0.9849	0.0159
90.0	0.9957	0.0121
92.5	0.9963	0.0009
95.0	1.0000	0.0077
97.5	0.9930	0.0313
100.0	0.9674	0.0578
102.5	0.9026	0.1352
105.0	0.7721	0.3302
107.5	0.5618	0.5464
110.0	0.3605	0.7146
112.5	0.1991	0.8437
115.0	0.1199	0.9189
117.5	0.0596	0.9367
120.0	0.0436	0.9628
122.5	0.0230	0.9825
125.0	0.0209	0.9839
127.5	0.0148	0.9964
130.0	0.0082	0.9764
132.5	0.0157	0.9793
135.0	0.0113	0.9798
137.5	0.0065	0.9926
140.0	0.0080	0.9871
142.5	0.0118	0.9809
145.0	0.0221	1.0000
147.5	0.0000	0.9862
150.0	0.0048	0.9979

TABLE 2 Parameter Values From the Least-Squares Fit of the Data in Table 1 to the Extended Logistic Function of Eq 3

NOTE 1—Uncertainties represent 95 % confidence levels.

Parameter	Cr (Disappearance)	Ni (Appearance)
A	1.009 ± 0.0154	0.0046 ± 0.0231
A_s	0.000756 ± 0.000688	-0.00028 ± 0.00107
B	0.0103 ± 0.0168	0.9888 ± 0.0258
B_s	-0.000049 ± 0.000519	0.00004 ± 0.00077
X_0 (min)	108.132 ± 0.153	106.985 ± 0.231
D_0 (min)	2.846 ± 0.108	2.801 ± 0.167
Q (min^{-1})	-0.0341 ± 0.0175	-0.0445 ± 0.0276
Residual Standard Deviation, σ	0.005567	0.008481
Confidence Limits for σ	0.004502 < σ < 0.007379	0.006858 < σ < 0.01124

calibrated sputtering standard under the same sputtering conditions of ion energy, beam angle, current density, etc., as the interface measurement itself. In this way, time can be transformed into an equivalent depth derived from a standard material and this equivalent depth should be used in reporting the interface parameters and analysis results. Sputtering standards are available from the National Institute of Standards and Technology[9] (SRM 2135c), from the European Institute for Reference Materials and Measurements[10] (BCR 261), and from the Surface Analysis Society of Japan[11] (a multilayer GaAs/AlAs superlattice material).

9. Example of Interface Profile Data Analysis Using the Method Suggested

9.1 Depth-profile data obtained at an interface between chromium (Cr) and nickel (Ni) have been analyzed by fitting the extended logistic function to these data using least-squares techniques.[5] An analysis is reported in this standard of simulated data, based on the parameter values obtained from measurements of the Cr/Ni SRM available from NIST.[9] The simulated data consist of normalized Auger spectral intensities and include random, normal errors of magnitude comparable to those obtained from the actual Cr/Ni measurements. The simulated data are given in Table 1 and the results of the analyses of the Cr and Ni simulated Auger intensities are given in Table 2 and Fig. 2. The data in Table 1 can and should be used as a basis for comparison of different algorithms. The uncertainties presented for the parameters in Table 2 represent 95 % confidence limits assuming a normal distribution of errors.

10. Keywords

10.1 depth-profile interface data; linescan interface data; logistic function

[9] Information on standard reference materials from the National Institute of Standards and Technology (NIST) is available from 100 Bureau Dr., Stop 1070, Gaithersburg, MD 20899-1070, http://ts.nist.gov/measurementservices/referencematerials/index.cfm.

[10] Information on certified reference materials from the European Institute for Reference Materials and Measurements is available from European Commission, Joint Research Centre, Institute for Reference Materials and Measurements, Retieseweg 111, B-2440 Geel, Belgium, http://www.irmm.jrc.be.

[11] Information on the GaAs/AlAs certified reference material can be obtained from the Surface Analysis Society of Japan at http://www.sasj.jp/eng-index.html.

APPENDIX

(Nonmandatory Information)

X1. FITTING OF DEPTH PROFILE AND LINESCAN DATA TO THE LOGISTIC FUNCTION BY MEANS OF A SPECIALIZED COMPUTER ALGORITHM, LOGISTIC FUNCTION PROFILE FIT (LFPF)

X1.1 Scope

X1.1.1 Appendix X1 describes a specialized computer algorithm and supporting software (LFPF) developed for the fitting of depth profile and linescan interface data to the extended logistic function in order to determine the parameters of this fitted function. These parameters characterize the shape of the interface region and so define the interface width, its asymmetry, and its depth from the original surface or its width along a scanned line.

X1.2 Significance and Use

X1.2.1 LFPF has been developed to fit interface profile data to the extended logistic function. The specifically written least-squares procedure used in LFPF results in a rapid and reliable analysis. An important feature of LFPF is that it does not require initial estimates to be made of the parameters; it is, therefore, simple and easy to use and can run without operator intervention. LFPF is robust in handling a wide variety of data of sigmoidal character and can deal effectively with extremely sharp profiles, noisy data, and incomplete profiles. It can also identify pronounced outliers.

X1.2.2 LFPF has been extensively tested on a variety of interface profile data; it has been found able to fit such data to the extended logistic function to within the measurement uncertainty.

X1.2.3 LFPF is a suitable implementation procedure for use with this practice.

X1.3 Description of the Procedure, LFPF

X1.3.1 LFPF has been written in Microsoft Visual Basic-.Net, an object oriented programming language that makes full use of the Microsoft Windows graphical user interface. It has been tested and found to run satisfactorily on computers using Microsoft Windows XP and Vista operating systems.

X1.3.2 LFPF is available for download together with accompanying documentation and instructions for use from NIST.[12]

X1.3.3 LFPF operates on ASCII text files created by the user or data entered directly into the program from the keyboard by the user. The data is in the form of tables whose rows consist of an independent variable, X, and up to 4 corresponding values of a dependent variable, Y, or a weighting factor to be used in the least squares fit, or a combination thereof. While the program can analyze poorly structured data, the statistics provided by the program are most reliable if the data consist of more than three values in each of the asymptotic regions and five values in the interface region.

X1.3.4 LFPF provides statistical uncertainties on the parameters of the logistic function allowing assessment and comparison of data quality from different laboratories.

X1.4 Description of the Fitting Procedure Used in LFPF

X1.4.1 Data in the form of X, Y pairs are fit by the method of least-squares to the extended logistic function:

$$Y = [A + A_s(X - X_0)]/(1 + e^z) \quad \text{(X1.1)}$$

$$+ [B + B_s(X - X_0)]/(1 + e^{-z})$$

where:

$$z = (X - X_0)/D, \text{ and } D = 2D_0/[1 + e^{Q(X - X_0)}] \quad \text{(X1.2)}$$

X1.4.1.1 Because these equations are non-linear functions of the three interface region parameters, X_0, D_0, and Q, the least-squares fit requires an iterative solution. Consequently, Y, as expressed above is expanded in a Taylor series about the current values of the parameters and the Taylor series is terminated after the first (that is, linear) term for each parameter. $Y_{obs} - Y_{calc}$ is fit 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.

X1.4.2 Initial estimates of the values of the parameters are calculated in LFPF automatically by one of three methods, selected because they were found to be least prone to false starts in situations of poorly structured data. The user has some control over the calculation of initial estimates in cases of poorly structured data.

X1.4.3 *The Least-Square Analysis*—A cycle of up to p iterations is executed in which, at the end of each iteration, the parameters are updated before the next iteration is performed. The number of iterations p is chosen on the basis of experience with particular classes of data. If p is selected to be a prime number, oscillations between two or three local minima can be identified by performing repeated multiples of p iterations. Generally, if convergence takes longer than eleven iterations, the solution is unstable in the sense that all of the parameters cannot be determined from the data. In most cases, instability of the fit can be interpreted by the program and the source of the instability removed by varying one fewer parameter in the least-squares fit. Messages keep the user informed of these situations. The confidence limits for the logistic curve calculated from the parameters of the least-squares fit are directly determined in LFPF.

X1.4.4 Situations with few data in the transition region can be accommodated by LFPF but with some loss of statistical significance.

[12] The LFPF software and its documentation can be downloaded from the web site of the Surface and Microanalysis Science Division of NIST at http://www.nist.gov/cstl/surface/lfpf.cfm.

X1.4.5 *Post-Fitting Tests*—Following the cycle of p iterations, several tests are performed to judge the quality of the fit, to test the assumption of the determinability of X_0, D_0, and Q, and the determinability of the asymptotic parameters A_s, B_s. If a test is failed, the analysis is repeated holding certain parameters constant. Analysis notes provided by the program describe actions taken by the program.

X1.4.5.1 The philosophy underlying the performance of the post-fitting tests is that the parameters A_s, B_s, and Q are of less interest in the analysis of the logistic profile than the parameters D_0 and X_0. In general (but not always), the former are of a heuristic nature and have little basis in the choice of the logistic function as a descriptor of an interface profile.

X1.4.6 *Outlier Identification and Rejection*—If directed to do so, LFPF will, following completion of analysis, identify outliers based on the assumption of a normal distribution of errors in the data and the confidence level specified by the user (the default being 95%.) The standardized residuals are used for the identification of the outliers. A standardized residual is the number of standard deviations by which $Y_{obs} - Y_{calc}$ differs from its expected value of zero, that is, the value of $Y_{obs} - Y_{calc}$ divided by the standard deviation of $Y_{obs} - Y_{calc}$.

X1.4.7 *Confidence Limits and Error Bars*—If directed to do so, LFPF will, following completion of analysis, display error bars equal to the confidence limits for each of the data or draw confidence intervals for the least squares profile, or both.

X1.5 Analysis Procedure Using LFPF

X1.5.1 LFPF is used in an interactive configuration for the analysis of interface data. With the graphical user interface, the user can select the following:

X1.5.1.1 Which data files are to be analyzed,

X1.5.1.2 Which parameters are to be varied,

X1.5.1.3 Which data are to be included in the analysis, and

X1.5.1.4 The results of a least-squares fit (the graphical display or the parameter table, or both) can be saved to the Windows clipboard for subsequent pasting into word processors.

X1.5.2 A user manual is included with the downloaded program and contains detailed descriptions of the program functionality, program outputs, and the full mathematical description of the analysis suitable for designing a similar program.

X1.5.3 Sample data files of test data, including the data file described above in this practice, accompany the program and may be used to evaluate program performance as well as for familiarization in the use of LFPF.

X1.6 Results of the Analysis

X1.6.1 The final results of an analysis of a depth profile or a linescan obtained with LFPF include the original data, 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.

X1.6.2 Use of these parameters to characterize the interface profile has been described in Section 7 of this practice.

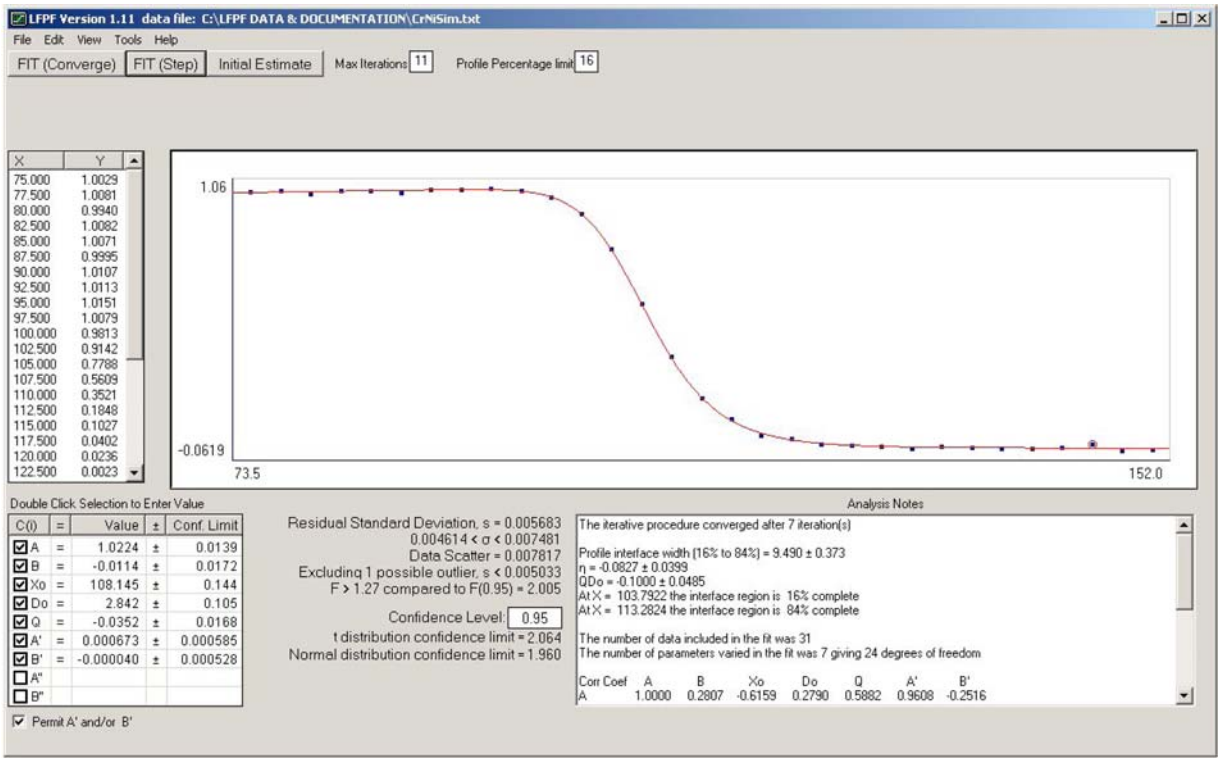
X1.7 Summary Demonstration of LFPF

X1.7.1 On initiating the program, the user is presented with instructions for entering profile data to be analyzed.

X1.7.2 After data entry and, if necessary, editing, a graph of the data is displayed along with "buttons" for initiating the analysis, text boxes for setting program operation parameters, a list of the original data, and a table of parameters to be varied. Following the least squares fit, the profile calculated from the least squares fit parameters is drawn through the data, the values of the parameters along with their uncertainties are displayed along with the overall statistics of the least squares fit and additional information about the analysis is printed in a text box labeled "Analysis Notes" as in Fig. X1.1:

X1.7.3 The analysis displayed in Fig. X1.1 also included a request to identify outliers, that is, data lying outside the 95 % (default value) confidence limits. This analysis also includes the statistics that would result if the outlier were excluded from the analysis.

X1.7.4 Many optional features including copying results, displaying additional statistics, remembering and displaying a previous analysis are available on the drop down menus.



NOTE 1—The *X*-axis is sputtering time and the *Y*-axis is the normalized Cr Auger signal.

FIG. X1.1 Results of a Least-Squares Analysis of Cr Disappearance in a Simulated Cr-Ni Interface