Designation: E 1636 – 94 (Reapproved 1999)

Standard Practice for Analytically Describing Sputter-Depth-Profile Interface Data by an Extended Logistic Function[1]

This standard is issued under the fixed designation E 1636; 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 covers a systematic method for analyzing sputter-depth-profile interface data and for accurately characterizing the shape of the interface region. Interface profile data are described with an appropriate analytic function; the parameters of this function define the interface width, its asymmetry, and its depth from the original surface. The use of this practice is recommended in order that the shapes of composition profiles of interfaces acquired with different instruments and techniques on different materials can be unambiguously compared and interpreted.

1.2 This practice is intended to be used to describe the shape of depth profile data obtained at an interface between two dissimilar materials for that case in which the measured concentration of the outer material goes from 100 to 0 % and the inner material goes from 0 to 100 %.

1.3 *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:*

E 673 Terminology Relating to Surface Analysis[2]

E 1127 Guide for Depth Profiling in Auger Electron Spectroscopy[2]

E 1162 Practice for Reporting Sputter Depth Profile Data in Secondary Ion Mass Spectrometry (SIMS)[2]

E 1438 Guide for Measuring Widths of Interfaces in Sputter Depth Profiling Using SIMS[2]

3. Terminology

3.1 *Definitions*—For definitions of terms used in this practice, see Terminology E 673.

3.2 *Definitions of Terms Specific to This Standard:*

3.2.1 Throughout this practice, the regions of the *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 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 sputtered depth.

4. Summary of Practice

4.1 Sputter depth profile interface data (composition versus depth) is fitted to an analytic function, an extended form of the logistic function, in order to describe the shape of such interface profiles.[3] Least-squares fitting techniques are employed to determine the values of the parameters of this extended logistic function which characterize the shape of the interface. Interface width, depth, and asymmetry are determined by 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 E 1127 and Practice E 1162). 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 E 1438), it is necessary to define the shape of the entire interface profile with a single analytic function.

5.2 Although no general physical model currently exists for describing the shape of interface sputter-depth profiles, interface profiles do have a sigmoidal shape characteristic of the cumulative logistic distribution. Use of such a logistic function is physically plausible and is superior to other functions (for example, polynomials) that have heretofore been used for

---

[1] This practice is under the jurisdiction of ASTM Committee E-42 on Surface Analysis and is the direct responsibility of Subcommittee E42.08 on Ion Beam Sputtering.

Current edition approved Sept. 15, 1994. Published November 1994.

[2] *Annual Book of ASTM Standards*, Vol 03.06.

[3] 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,* , p. 1666, 1986.

interface profile analysis in that it contains the minimum number of parameters for describing interface shapes.

5.3 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 in a reproducible and unambiguous way.

6. Description of the Analysis

6.1 *Logistic Function Data Analysis*—In its simplest form, the logistic 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. The logistic function was first named and applied to population growth in the last century by Verhulst.[4] The logistic function as a distribution function and growth curve has been extensively reviewed by Johnson and Kotz.[5] Interface profile data is fitted to an extended form of the logistic function:

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

where:

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

and:

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

6.1.1 Y is 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. Pre-interface and post-interface elemental surface concentrations are described by the parameters A and B, respectively, the parameters A_s and B_s are introduced to account for time dependent instrumental effects. X_o is the midpoint of the interface region (interface depth or time). The scaling factor D_o is the characteristic depth for sputtering through the interface region; Q, an asymmetry parameter, is a measure of the difference in curvature in the pre- and post-interface ends of the interface region. All measures of the interface width can be determined from D_o and Q.

6.2 Fitting of interface profile data to the above functions, Eq 3 , can be accomplished by using least-squares techniques. Because these equations are non-linear functions of the three transition-region parameters, X_o, D_o, 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 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. Values for interface width, depth, and asymmetry can be calculated from the parameters of the fitted logistic function.

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

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 typical interface profiles, it is usual to assume that both of these slopes are zero. Two more parameters, $D_o$and X_o, define the slope and position of the transition region. In addition, an asymmetry parameter Q that causes the width parameter to vary logistically from O to $2D_o$, is introduced as a measure of the difference in curvature in the pre- and post-transition ends of the transition region. If $Q <$ O, the pre-transition region has the greatest (sharpest) curvature. If $Q >$ O, the post-transition region has the greatest curvature. If $Q =$ O, $D = D_o$ and the transition profile is symmetric. The parameter Q has the dimensions of $1/X$ whereas D_o has the dimensions of X. The product QD_o is dimensionless and is a measure of the asymmetry of the profile independent of its width. If the absolute magnitude of $QD_o$is less than 0.1, the asymmetry in the transition profile should be barely discernible.

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) required for the decay or growth curve to progress from a fraction f of completion to $(1 - f)$ of completion. For the case where $Q =$ O, I_f is proportional to D_o and is given by the simple formula:

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

so that, for example, the traditional 16 to 84 % interface width is 3.32 D_o.

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:

$$X_f = X_o + 2\,D_o \ln[f/(1 - f)]/[1 + e^{Q(X_f - X_o)}] \tag{7}$$

---

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

[5] Johnson, N. L. and Kotz, S., “Distributions in Statistics: Continuous Univariate Distributions,” Houghton Mifflin Co., Boston, *2*, Chapter 22, 1970.

and:

$$X_{(1-f)} = X_o + 2\,D_o\,1n\,[(1-f)/f]/[1 + e^{Q(X_{1-f}-X_o)}] \qquad (8)$$

X_f and $X_{(1-f)}$ can be evaluated most readily by Newton's method of successive approximations.

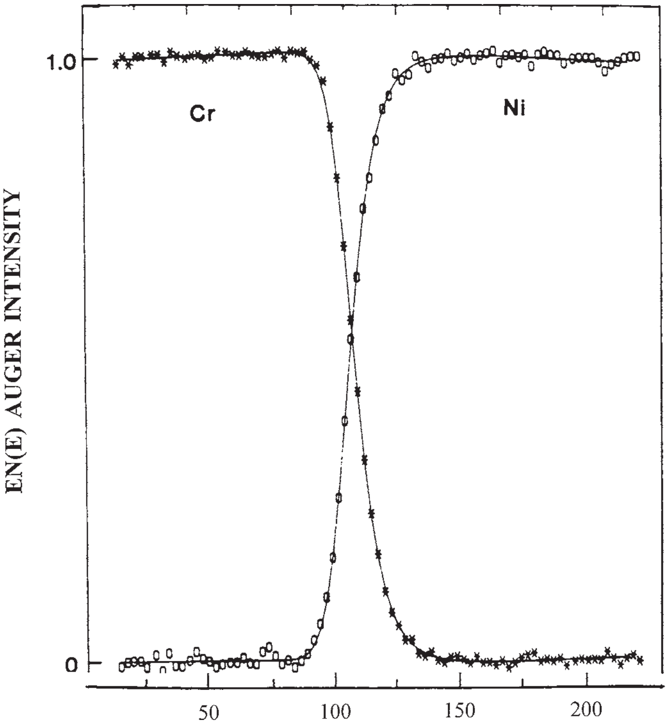
8. Reporting of Results

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_o, D_o, Q) together with their uncertainties, the standard deviation of the fit, and an interface width obtained from D_o and Q that is based on some accepted definition (for example, 16 to 84 % concentration change).

8.2 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 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 (SRM 2136)[6] and from the UK National Physical Laboratory (No. S7B83).[7]

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

9.1 Sputter-depth-profile data obtained at an interface between Cr and Ni has been analyzed by fitting the extended logistic function to this data using least-squares techniques. The results of this analysis are presented in Fig. 1; the solid lines are calculated values from Eq 3 . A separate analysis was done for each constituent to determine the parameters of the fit; these are listed in Table 1. Comparison of the chromium and nickel parameters indicates the high precision attainable in describing the profile shape and in determining sputtered depth (and, therefore, interface width) with this analysis method.



NOTE 1—The solid lines are the calculated values from Eq 3 . Parameters of the fit are given in Table 1.

FIG. 1 Typical Depth Profile of Chromium Through a Chromium (x) and Nickel (o) Interface

TABLE 1 Profile Parameters for a Typical Chromium/Nickel Interface

Chromium (Disappearance Profile)	Nickel (Appearance Profile)
A = 14893 ± 43	A = −88 ± 47
A_s = 4.59 ± 1.32	A_s = 1.65 ± 1.46
B = −168 ± 69	B = 10656 ± 73
B_s = 4.43 ± 1.81	B_s = −2.19 ± 1.90
X_o = 108.2 ± 0.1 min	X_o = 107.3 ± 0.1 min
D_o = 2.86 ± 0.03 min	D_o = 2.80 ± 0.05 min
Q = −0.045 ± 0.006 min^{-1}	Q = −0.047 ± 0.008 min^{-1}
72 data points, 20 in the interval	73 data points, 18 in the interval
Standard Deviation in Y = 79.1	Standard Deviation in Y = 89.9

10. Keywords

10.1 logistic function; sputter-depth-profile interface data

---

[6] Available from National Institute of Standards and Technology, (NIST) Gaithersburg, MD 20899.

[7] Available from UK National Physical Laboratory, Teddington, Middlesex, UK TW 10LW.