PHYSICAL REVIEW B VOLUME 43, NUMBER 13 1 MAY 1991

Penetration of an electron beam in a thin solid film: The influence of backscattering from the substrate

Maurizio Dapor
Divisione Scienza dei Materiali, Istituto per la Ricerca Scientifica e Tecnologica, I-38050 Povo, Trento, Italy
(Received 24 July 1990)

The fractions of absorbed, backscattered, and transmitted electrons bombarding a thin solid film are calculated as functions of the film thickness both in the absence and in the presence of a substrate. The depth distribution of the absorbed electrons has also been calculated.

I. INTRODUCTION

The interaction of an electron beam with a solid target has been extensively studied since 1930.[1-3] An excellent review of the early works about this subject has been given by Birkhoff.[4] More recently, several theoretical models and experimental data have been proposed.[5-16]

In the past few years several Monte Carlo simulations have been described by a number of researchers[17-33] in order to approach the problem numerically. The most recent investigations have been performed for keV electrons due to the increasing interest in material analysis techniques such as electron probe microanalysis,[19,27] electron-energy-loss spectroscopy,[20] Auger electron spectroscopy,[29-32] etc.

The numerical approaches are very powerful in calculating, in particular, the fractions of absorbed, backscattered, and transmitted electrons bombarding a thin solid film but does not give any general formula. In this paper the fractions of absorbed, backscattered, and transmitted electrons bombarding a thin solid film are calculated as functions of the film thickness both in the absence and in the presence of a substrate. The results regarding thin films in the absence of a substrate are in very good agreement with the Cosslett and Thomas experimental data.[9] On the other hand, the equations regarding a thin film deposited on the top of a substrate of a different material can be used to evaluate the film thickness just by measuring the backscattering fraction.

II. DEFINITIONS AND PROPERTIES

When a particle beam impinges on a solid target, a fraction f_A of the beam is absorbed, a fraction f_B is backscattered, and the remaining fraction f_T is transmitted. The sum of these fractions is equal to 1 and each of them lies in the range 0–1. Their value depends on the thickness s of the target. There exists, in particular, a thickness R so that, for each $s>R$, the fraction of transmitted particles f_T is 0 while that of backscattered ones is equal to the so-called backscattering coefficient r. Both the maximum penetration range R and the backscattering coefficient r depend on the material, on the primary energy E_0 of the particle beam, and on the kind of particles.

The fractions f_A, f_B, and f_T depend on s through the function $\xi=s/\lambda(E)$ where $\lambda(E)$ is the mean free path of a particle of energy E, and E is the beam mean energy after a path of length s inside the solid. In the continuum-energy-loss approximation, when a particle has traveled in the solid along a path equal to R, it has completely lost its energy. Since $\lambda=0$ for $E=0$, then $\xi\to\infty$ for $s\to R$. On the other hand, since $\lambda(E_0)$ has a finite value, then $\xi\to 0$ for $s\to 0$. The function ξ, expanding the thickness range $0\le s<R$ to the extended range $0\le\xi<\infty$, takes into account the mean energy lost in the solid target by the particle beam.

The dependence of f_A, f_B, and f_T on ξ will be found taking into account that

$$f_A(\xi)+f_B(\xi)+f_T(\xi)=1 \tag{1}$$

and that

$$\text{for } \xi\to 0 \text{ then } f_A\to 0,\ f_B\to 0,\ f_T\to 1 , \tag{2}$$

while

$$\text{for } \xi\to\infty \text{ then } f_A\to 1-r,\ f_B\to r,\ f_T\to 0 . \tag{3}$$

III. THEORY OF ABSORPTION, BACKSCATTERING, AND TRANSMISSION

Let us suppose known values for f_A, f_B, and f_T for a film of thickness s bombarded by a particle beam of primary energy E_0. We are interested in the values of these fractions when the film thickness is incremented by Δs. Let us indicate with $\Delta\xi$ the increment of the extended thickness given by

$$\Delta\xi=\xi(s+\Delta s)-\xi(s) . \tag{4}$$

The fraction of particles absorbed by the film of thickness $s+\Delta s$,

$$f_A[\xi(s+\Delta s)]=f_A(\xi+\Delta\xi) ,$$

is given by the fraction absorbed by ξ, plus the fraction transmitted through ξ and absorbed by $\Delta\xi$, plus the fraction that, once transmitted through ξ and backscattered by $\Delta\xi$, is absorbed by ξ and so on. Reasoning in such a way, one obtains the following infinite sum:

$$
\begin{aligned}
f_A(\xi+\Delta\xi)=&f_A(\xi)+f_T(\xi)f_A(\Delta\xi)+f_T(\xi)f_B(\Delta\xi)f_A(\xi)\\
&+f_T(\xi)f_B(\Delta\xi)f_B(\xi)f_A(\Delta\xi)+f_T(\xi)f_B(\Delta\xi)f_B(\xi)f_B(\Delta\xi)f_A(\xi)+\cdots\\
=&f_A(\xi)+f_A(\xi)f_T(\xi)f_B(\Delta\xi)\sum_{n=0}^{\infty}[f_B(\xi)f_B(\Delta\xi)]^n+f_T(\xi)f_A(\Delta\xi)\sum_{n=0}^{\infty}[f_B(\xi)f_B(\Delta\xi)]^n .
\end{aligned}
$$

Reasoning in the same way, we obtain

$$
\begin{aligned}
f_B(\xi+\Delta\xi)=&f_B(\xi)+f_T(\xi)f_B(\Delta\xi)f_T(\xi)\\
&+f_T(\xi)f_B(\Delta\xi)f_B(\xi)f_B(\Delta\xi)f_T(\xi)+\cdots\\
=&f_B(\xi)+f_T^2(\xi)f_B(\Delta\xi)\sum_{n=0}^{\infty}[f_B(\xi)f_B(\Delta\xi)]^n
\end{aligned}
$$

and

$$
\begin{aligned}
f_T(\xi+\Delta\xi)=&f_T(\xi)f_T(\Delta\xi)\\
&+f_T(\xi)f_B(\Delta\xi)f_B(\xi)f_T(\Delta\xi)+\cdots\\
=&f_T(\xi)f_T(\Delta\xi)\sum_{n=0}^{\infty}[f_B(\xi)f_B(\Delta\xi)]^n .
\end{aligned}
$$

Now, since

$$\sum_{n=0}^{\infty}[f_B(\xi)f_B(\Delta\xi)]^n=\frac{1}{1-f_B(\xi)f_B(\Delta\xi)} ,$$

then

$$f_A(\xi+\Delta\xi)=f_A(\xi)+\frac{f_A(\xi)f_B(\Delta\xi)f_T(\xi)+f_A(\Delta\xi)f_T(\xi)}{1-f_B(\xi)f_B(\Delta\xi)} , \tag{5}$$

$$f_B(\xi+\Delta\xi)=f_B(\xi)+\frac{f_T^2(\xi)f_B(\Delta\xi)}{1-f_B(\xi)f_B(\Delta\xi)} , \tag{6}$$

$$f_T(\xi+\Delta\xi)=\frac{f_T(\xi)f_T(\Delta\xi)}{1-f_B(\xi)f_B(\Delta\xi)} . \tag{7}$$

Let us consider the case in which $\Delta\xi=\infty$ and, as a consequence,

$$f_A(\xi+\Delta\xi)=f_A(\Delta\xi)=1-r$$

and $f_B(\Delta\xi)=r$. Equation (5) becomes, in such a case:

$$1-r=f_A(\xi)+\frac{f_A(\xi)rf_T(\xi)+(1-r)f_T(\xi)}{1-rf_B(\xi)} .$$

Taking into account Eq. (1) in order to eliminate $f_A(\xi)$, the following relationship between $f_B(\xi)$ and $f_T(\xi)$ follows:

$$f_T^2=f_B^2-2\mu f_B+1 , \tag{8}$$

where

$$\mu=\frac{1+r^2}{2r} . \tag{9}$$

Equation (8) can also be obtained by using (6) in the same limit. Once (8) has been substituted in (6) one can conclude that

$$f_B(\xi+\Delta\xi)=\frac{f_B(\xi)-2\mu f_B(\xi)f_B(\Delta\xi)+f_B(\Delta\xi)}{1-f_B(\xi)f_B(\Delta\xi)} . \tag{10}$$

The substitution of (8) in (5), once one takes into account (7) and (10), gives Eq. (1).

By using (8) it is easy to see that

$$\frac{1-f_T}{f_B}=\frac{2\mu-f_B}{1+f_T}$$

and, as a consequence,

$$\mu=\lim_{\xi\to 0}\left[\frac{1-f_T(\xi)}{f_B(\xi)}\right] . \tag{11}$$

Therefore, r can be found not only by measuring f_B for a bulk but also by measuring f_B and f_T for a very thin film.

Now we suppose that our fractions $f_A(\xi)$, $f_B(\xi)$, and $f_T(\xi)$ are differentiable for all the value of ξ. Let us indicate, in particular, with σ, the derivative of $f_B(\xi)$ calculated in the origin

$$\sigma=\lim_{\xi\to 0}\left[\frac{f_B(\xi)}{\xi}\right]=\frac{df_B}{d\xi}(\xi=0) \tag{12}$$

[remember that $f_B(0)=0$].

By using Eq. (10) [or (6)], it is easy to see that

$$\frac{f_B(\xi+\Delta\xi)-f_B(\xi)}{\Delta\xi}=\frac{f_B(\Delta\xi)}{\Delta\xi}\frac{f_B^2(\xi)-2\mu f_B(\xi)+1}{1-f_B(\xi)f_B(\Delta\xi)} \tag{13}$$

and, therefore,

$$\frac{df_B}{d\xi}=\sigma(f_B^2-2\mu f_B+1)=\sigma f_T^2 . \tag{14}$$

Equation (8) gives

$$\frac{df_T/d\xi}{df_B/d\xi}=\frac{f_B-\mu}{f_T} \tag{15}$$

and, then,

$$\frac{df_T}{d\xi}=\sigma f_T(f_B-\mu) . \tag{16}$$

Since

$$\frac{df_A}{d\xi}=-\frac{df_B}{d\xi}-\frac{df_T}{d\xi} , \tag{17}$$

then

$$\frac{df_A}{d\xi}=\sigma f_T(\mu-f_B-f_T) . \tag{18}$$

Equation (14) is equivalent to

$$\frac{df_B}{f_B-(1/r)}-\frac{df_B}{f_B-r}=2\nu\sigma d\xi , \tag{19}$$

where

$$\nu=\frac{1-r^2}{2r} . \tag{20}$$

The integration of Eq. (19) with the boundary condition $f_B(0)=0$ gives

$$f_B(\xi)=r\frac{1-\exp(-2\nu\sigma\xi)}{1-r^2\exp(-2\nu\sigma\xi)} . \tag{21}$$

By using (8) [or (14)] and (21), it follows that

$$f_T(\xi)=\frac{1-r^2}{1-r^2\exp(-2\nu\sigma\xi)}\exp(-\nu\sigma\xi) \tag{22}$$

and, by using Eq. (1), one concludes

$$f_A(\xi)=(1-r)\frac{r\exp(-2\nu\sigma\xi)-(1+r)\exp(-\nu\sigma\xi)+1}{1-r^2\exp(-2\nu\sigma\xi)} . \tag{23}$$

IV. THE INFLUENCE OF THE SUBSTRATE

Let us now consider a system composed of a film of the material x of thickness s deposited on a substrate of the material y. In the following, the superscripts x and y will indicate the material considered (for example, R^x and R^y will indicate the maximum penetration ranges in x and y, respectively). We assume that the thickness of the substrate is larger than R^y, namely the substrate is a bulk for the primary energy considered.

We expect that the maximum penetration range will be some combination of R^x and R^y depending on the film thickness: in particular, when $s\to 0$, then this combination will approach R^y and when $s\to R^x$, the combination approaches R^x. We will indicate with $h_A(\xi)$ the fraction of electrons absorbed by the film, with $h_B(\xi)$ the fraction of electrons backscattered by the system, and with $h_T(\xi)$ the fraction of electrons transmitted across the interface between the film x and the substrate y.

These fractions are obviously different from the corresponding $f_A(\xi)$, $f_B(\xi)$ and $f_T(\xi)$ relative to a film of x without substrate because of the influence of backscattering from the y substrate. Obviously, each h fraction lies in the range (0–1) and the following equation holds:

$$h_A(\xi)+h_B(\xi)+h_T(\xi)=1 . \tag{24}$$

If we indicate with r^x and r^y the backscattering coefficients of, respectively, x and y, we expect that

$$\text{for } \xi\to 0 \text{ then } h_A\to 0,\ h_B\to r^y,\ h_T\to 1-r^y , \tag{25}$$

while

$$\text{for } \xi\to\infty \text{ then } h_A\to 1-r^x,\ h_B\to r^x,\ h_T\to 0 . \tag{26}$$

V. CALCULATION OF THE RELATIONSHIP BETWEEN THE *h* AND THE *f* FRACTIONS

In order to calculate the relationship between the h and the f fractions, some simple consideration has to be done about the contribution given to the h fractions by backscattering from the y substrate. Let us consider the absorbed fraction h_A. First of all, a fraction f_A is absorbed by the film, then a fraction f_Tr^y goes back across the interface, and so a fraction $f_Tr^yf_A$ is also absorbed, then a fraction $f_Tr^yf_B$ is reflected back in the y substrate and so a fraction $f_Tr^yf_Br^yf_A$ is also absorbed. In such a way one can write down the following infinite sum of contributions to the absorbed fraction:

$$\begin{aligned} h_A&=f_A+f_Tr^yf_A+f_Tr^yf_Br^yf_A+f_Tr^yf_Br^yf_Br^yf_A+\cdots\\ &=f_A\{1+f_Tr^y[1+f_Br^y+(f_Br^y)^2+\cdots]\}\\ &=f_A[1+f_Tr^y/(1-f_Br^y)] . \end{aligned} \tag{27}$$

In a similar way one can calculate the fraction of backscattered and transmitted electrons:

$$\begin{aligned} h_B&=f_B+f_Tr^yf_T+f_Tr^yf_Br^yf_T+f_Tr^yf_Br^yf_Br^yf_T+\cdots\\ &=f_B+(f_T)^2r^y[1+f_Br^y+(f_Br^y)^2+\cdots]\\ &=f_B+(f_T)^2r^y/(1-f_Br^y) , \end{aligned} \tag{28}$$

$$\begin{aligned} h_T&=f_T-f_Tr^yf_A-f_Tr^yf_T-f_Tr^yf_Br^yf_A-f_Tr^yf_Br^yf_T-\cdots\\ &=f_T-f_Tr^y+f_Tr^yf_B-f_Tr^yf_Br^y+f_Tr^yf_Br^yf_B\dot{-}\cdots\\ &=f_T[1+f_Br^y+(f_Br^y)^2+\cdots]-f_Tr^y[1+f_Br^y+(f_Br^y)^2+\cdots]\\ &=f_T(1-r^y)/(1-f_Br^y) . \end{aligned} \tag{29}$$

Equations (27)–(29) allow one to calculate the changing in absorption, backscattering, and transmission due to the presence of the substrate.

VI. CASE IN WHICH THE MATERIAL CONSTITUTING THE OVERLAYER IS THE SAME AS THE SUBSTRATE: DEPTH DISTRIBUTION OF THE ABSORBED ELECTRONS

Let us consider now the particular case in which the material constituting the film is the same as the substrate. In such a case we can avoid all the superscripts and the interface is now only an imaginary boundary at the depth s below the surface, then $h_B=r$ and (28) becomes

$$h_B=r=f_B+f_T^2 r/(1-f_B r) . \tag{30}$$

Equations (27) and (29) read, in such a case,

$$\begin{aligned} h_A&=f_A[1+f_T r/(1-f_B r)] \\ &=(1-r)\{[f_A+f_B(1-r)]/(1-f_B r)\} , \end{aligned} \tag{31}$$

$$h_T=f_T(1-r)/(1-f_B r) . \tag{32}$$

[The third member in (31) has been obtained by making use of (30).] Equations (31) and (32) are the same equations given by Cosslett and Thomas[9] and express the following facts remarked by these authors.

(1) The number of electrons absorbed in a surface layer of a bulk of a given material is greater than the number of electrons absorbed in a film of equal thickness.

(2) The number of transmitted electrons across an imaginary boundary below the surface of a bulk of a given material is less than the number of electrons transmitted through a film of equal thickness.

By substituting Eqs. (21)–(23) in Eqs. (30)–(32) we obtain

$$h_A=(1-r)[1-\exp(-\nu\sigma\xi)] , \tag{33}$$

$$h_B=r , \tag{34}$$

$$h_T=(1-r)\exp(-\nu\sigma\xi) . \tag{35}$$

The derivative of (33) gives the depth distribution of the absorbed electrons as

$$\frac{dh_A}{ds}=\nu\sigma(1-r)\exp(-\nu\sigma\xi)d\xi/ds . \tag{36}$$

VII. RESULTS

Equations (21)–(23) give the dependence of f_A, f_B, and f_T by the extended thickness ξ. The comparison with the available experimental data can only be performed once the relationship between the extended thickness ξ and the real thickness s is known. This is the disadvantage of the formulas derived in this paper because they require the knowledge of such a relationship. This relationship will depend both on the energy-loss law and on the energy dependence of the mean free path of the particle beam inside the solid.

We wish to study the case in which the energy-loss law is given by

$$\begin{aligned} R&=K_R E_0^p , \\ E^p&=(1-u)E_0^p , \end{aligned} \tag{37}$$

where K_R is a constant dependent only on the material constituting the target, the exponent p does not depend either on the material or the primary energy, u is the reduced depth s/R, and E_0 is the primary energy. The energy dependence of the mean free path we wish to consider here is given by

$$\lambda=K_\lambda E^p , \tag{38}$$

where K_λ is a constant dependent only on the material.

Equations (37) and (38) contain all the information concerning the energy lost by the particle beam along its path inside the solid: their origin can be found, for example, in Ref. 11. By using such equations, one easily concludes that

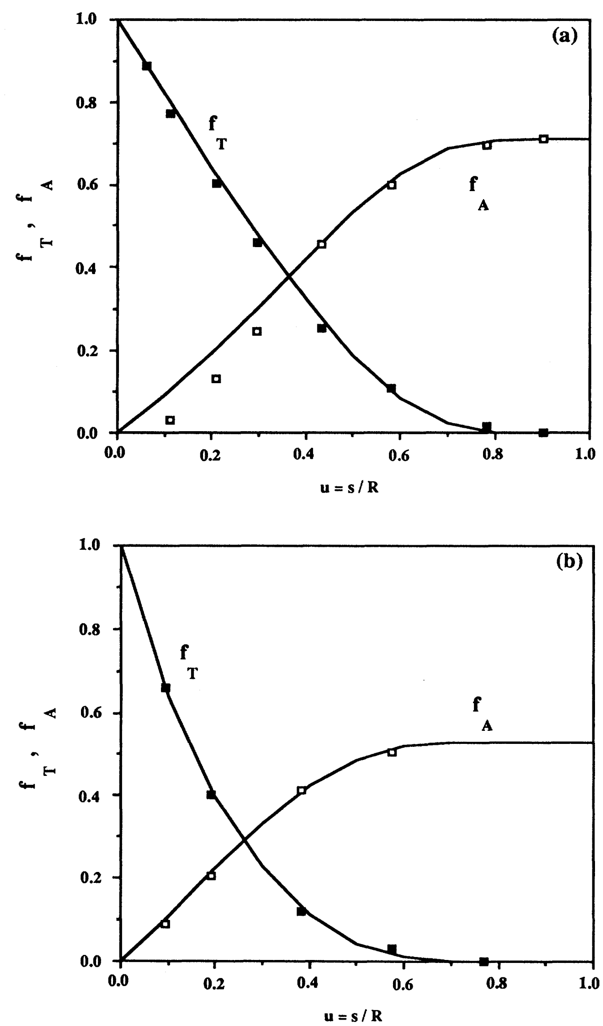

FIG. 1. Fractions of electrons absorbed (f_A) and transmitted (f_T) for (a) Cu and (b) Au thin films as functions of the reduced depth u. Solid lines are the theoretical trends while squares are the Cosslett and Thomas 10-keV experimental data (Ref. 9).

$$\xi = k\frac{u}{1-u} , \tag{39}$$

where $k = K_R / K_\lambda$ is a constant dependent only on the material.

Once (39) has been substituted in (21)–(23), the dependence of f_A, f_B, and f_T by the real thickness s is known if the backscattering coefficient r, the maximum penetration range R, and the product $k\sigma$, namely, the derivative of f_B in relation to u calculated for $u = 0$, are given. In Fig. 1 the absorbed and transmitted fractions as calculated by (23) and (22), respectively, are shown with $r = 0.29$, $R = 0.46$ μm, and $k\sigma = 1.0$ [Fig. 1(a)] and with $r = 0.47$, $R = 0.27$ μm, and $k\sigma = 3.5$ [Fig. 1(b)]. The Cosslett and Thomas experimental data[9] of a 10-keV electron beam bombarding a copper target [Fig. 1(a)] and a gold target [Fig. 1(b)] are also shown (the values of r, R and $k\sigma$ have been chosen in order to fit such experimental data).

Obviously, the particular choice of the energy loss and mean-free-path functional form is not dependent on the theory described by Eqs. (21)–(23). On the other hand, the agreement between theory and experiment indicates, in particular, that the energy-loss law given by Eq. (37) and the energy dependence of the mean free path given by Eq. (38) are suitable to describe the energy lost by an electron beam inside a solid target.

In particular, the depth distribution of the absorbed electrons, Eq. (36), becomes

$$\rho(u) = \frac{dh_A}{du} = \{ \nu\sigma k(1-r)\exp[-\nu\sigma\xi(u)] \} / (1-u)^2 . \tag{40}$$

The maximum of the distribution is found to be at the reduced depth $u = u_{\max} = 1 - \nu\sigma k/2$ and one can easily see that

$$\rho(u_{\max}) = \{ 4(1-r)\exp[-(2-\nu\sigma k)] \} / (\nu\sigma k) , \tag{41}$$

$$\rho(0) = (1-r)(\nu\sigma k) , \tag{42}$$

$$\rho(1) = 0 . \tag{43}$$

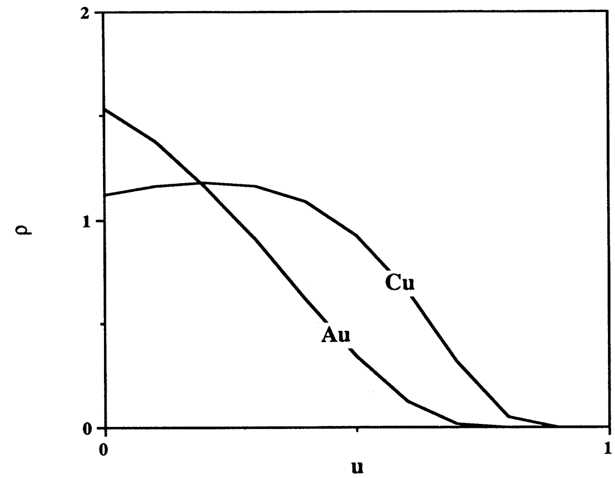

FIG. 2. Depth distribution of the electrons absorbed in a copper and in a gold target bombarded by a 10-keV electron beam.

For copper, $u_{\max} = 0.21$ while, for gold, $u_{\max} = -0.45$: this means that, for gold, ρ is a decreasing function having its maximum value in the origin (Fig. 2).

VIII. CONCLUSIONS

The fractions of absorbed, backscattered, and transmitted electrons bombarding a thin solid film have been calculated as functions of the film thickness both in the absence and in the presence of a substrate. The depth distribution of the absorbed electrons has also been calculated. The Cosslett and Thomas experimental data are in very good agreement with the results of the calculation regarding thin films without substrates.

ACKNOWLEDGMENTS

The author wishes to thank Dr. Fabio Marchetti for helpful comments and Susan Struthers for her skillful technical assistance in translating the manuscript.

[1]H. A. Bethe, Ann. Phys. (Leipzig) **5**, 325 (1930).
[2]G. Molière, Z. Naturforsch. **3A**, 78 (1948).
[3]H. A. Bethe, Phys. Rev. **89**, 1256 (1953).
[4]R. D. Birkhoff, in *Encyclopedia of Physics,* edited by S. Flügge (Springer-Verlag, Berlin, 1958), Vol. XXXIV, pp. 53–138.
[5]H. W. Streitwolf, Ann. Phys. (Leipzig) **3**, 183 (1959).
[6]G. D. Archard, J. Appl. Phys. **32**, 1505 (1961).
[7]L. Marton, J. A. Simpson, H. A. Fowler, and N. Swanson, Phys. Rev. **126**, 182 (1962).
[8]J. Quinn, Phys. Rev. **126**, 1453 (1962).
[9]V. E. Cosslett and R. N. Thomas, Br. J. Appl. Phys. **15**, 883 (1964); **16**, 779 (1965).
[10]M. Gryzinski, Phys. Rev. **138**, A336 (1965).
[11]K. Kanaya and S. Okayama, J. Phys. D **5**, 43 (1972).
[12]R. Mayol, J. D. Martinez, and F. Salvat, Nucl. Instrum. Methods Phys. Res. A **255**, 117 (1987).
[13]J. I. Goldstein, D. E. Newbury, P. Echlin, D. C. Joy, C. Fiori, and E. Lifshin, in *Scanning Electron and X-Ray Microanalysis* (Plenum, New York, 1984), pp. 72–78.
[14]J. C. Ashley, J. Electron Spectrosc. Relat. Phenom. **46**, 199 (1988).
[15]Z.-J. Ding and R. Shimizu, Surf. Sci. **222**, 313 (1989).
[16]M. Dapor, Phys. Lett. A **151**, 84 (1990).
[17]J. E. Leiss, S. Penner, and C. S. Robinson, Phys. Rev. **107**, 1544 (1957).
[18]J. F. Perkins, Phys. Rev. **126**, 1781 (1962).
[19]G. Love, M. G. C. Cox, and V. D. Scott, J. Phys. D **10**, 7 (1977).
[20]A. Desalvo, A. Parisini, and R. Rosa, J. Phys. D **17**, 2455 (1984).
[21]J. P. Ganachaud and M. Cailler, Surf. Sci. **83**, 498 (1979).
[22]J. P. Ganachaud and M. Cailler, Surf. Sci. **83**, 519 (1979).
[23]F. Salvat and J. Parellada, J. Phys. D **17**, 185 (1984).
[24]F. Salvat and J. Parellada, J. Phys. D **17**, 1545 (1984).
[25]F. Salvat, J. D. Martinez, R. Mayol, and J. Parellada, Comput. Phys. Commun. **42**, 93 (1986).

[26]A. F. Bielajew and D. W. O. Rogers, Nucl. Instrum. Methods Phys. Res. B **18**, 165 (1987).
[27]R. Shimizu, Y. Kataoka, T. Matsukawa, T. Ikuta, K. Murata, and H. Hashimoto, J. Phys. D **8**, 820 (1975).
[28]R. Shimizu, Y. Kataoka, T. Ikuta, T. Koshikawa, and H. Hashimoto, J. Phys. D **9**, 101 (1976).
[29]R. Shimizu, M. Aratama, S. Ichimura, and Y. Yamazaki, Appl. Phys. Lett. **31**, 692 (1977).
[30]S. Ichimura and R. Shimizu, Surf. Sci. **112**, 387 (1981).
[31]S. Ichimura, Ding Ze-Jun, and R. Shimizu, Surf. Interface Anal. **13**, 149 (1988).
[32]A. Jablonski, Surf. Interface Anal. **14**, 659 (1989).
[33]M. Dapor, Phys. Lett. A **143**, 160 (1990).