# BACKSCATTERING FACTOR FOR KLL AUGER YIELD FROM FILM-SUBSTRATE SYSTEMS

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## Introduction

The use of AES for estimating the thickness of an overlayer or film-substrate system was suggested earlier by Holloway[1]. Much work has been done since to study the Auger yield in depth profile measurements of various film-substrate systems experimentally[2,3,4,5] and by Monte Carlo simulation[4,6] and/or analytic[5] approach via the backscattering factor, R. As discussed by Jablonski and Powell[7] in a recent review, the Auger signal intensity originating from a layer of film ($Z_F$) with thickness $t_o$ sitting on a semi-infinite thick substrate ($Z_S$) is given by

$$I(t_o,Z_F,Z_S,E_P,E_b) = \int_0^{t_o} \frac{\Delta\Omega}{4\pi} I_o \, P_A \, \sigma(E_p) \, R_{FS} \, N \, Q \left( \frac{\lambda}{L} \right) \exp\left( -Z/(L \cos\alpha) \right) dZ \qquad (1)$$

where $\Delta\Omega$ is the solid angle subtended by the CMA detector, $I_o$ is the incident beam intensity, $P_A$ is the probability that an Auger transition follows the ionization of a core level, $\sigma(E_P)$ is the ionization cross-section, $R_{FS}$ is the film-substrate backscattering factor, N is the atomic density, $\lambda$ is the inelastic mean free path of Auger electron, Q is the correction parameter for elastic multiple scattering effects, L is the attenuation length and $\alpha$ the angle of incidence of the incoming primary electrons.

$R_{FS}$, an important basic correction factor in quantitative AES, gives the extra Auger yield due to backscattering of the primary electrons from the film-substrate. It is given in general by,

$$R_{FS}(t_o,Z_F,Z_S,E_P,E_b) = 1 + \frac{\cos(\alpha)}{I_o \, \sigma(E_P)} \int_{E_b}^{E_p} \int_0^{\frac{\pi}{2}} I_b(t_o,Z_F,Z_S,E,\theta) \, \sigma(E) \, \sec(\theta) \, dE \, d\theta \qquad (2)$$

where $I_b(t_O,Z_F,Z_S,E,\theta)$ is the film-substrate backscattered energy-angular distribution. $\theta$ is the backscattered angle taken with respect to the surface normal.

In the limit where $t_o \to \infty$, $R_{FS} = R_{Z_F}(E_P,E_b)$ and for $t_o \to 0$, $R_{FS} = R_{Z_S}(E_P,E_b)$. $R_{Z_F}$ and $R_{Z_S}$ are the backscattering factors for bulk film and substrate material respectively. From eq.(2), it can be seen that $R_{FS}$ is dependent on the scattering behavior of both the film and substrate material for intermediate thicknesses and is therefore important for the proper calculation of Auger intensity during depth profiling or overlayer measurement.

By normalizing eq.(1) to the bulk film intensity, the relation is now given by

$$I^N(t_o,Z_F,Z_S,E_P,E_b) = \frac{R_{FS}\{1 - \exp[-t_o/(L\cos\alpha)]\}}{R_{Z_F}} \qquad (3)$$

Using eq.(3) with the appropriate attenuation length L, $R_{FS}$ and $R_{Z_F}$, the relative depth intensity at film thickness $t_o$ can then be calculated. Our present work focusses on a comprehensive description of the change in $R_{FS}$ for KLL Auger yield with film thickness on various substrates and for different primary energies, hence to derive an analytic expression for calculating $R_{FS}$.

## Results and Discussion

We present here the results of film-substrate Monte Carlo simulations for C (KLL) on Al, Cu, and Au substrates and Al (KLL) on C, Cu, and Au substrates. Primary energies range from 2 to 40 keV. Correction factors were used firstly for modifying the screened Rutherford step length at lower energies especially below 5 keV and for high Z elements. Secondly film-substrate correction, as the electron traverses from one medium to another, was also taken into account by a simple ratio of the two elastic mean free path. Careful testing of the program in bulk and film-substrate cases show good agreement with the empirical backscattering results of August and Wernisch[10] and Hunger and Rogaschewski[11] respectively. Each $R_{FS}$ value is calculated using the well-known Gryzinski semi-empirical ionization cross-section. For each primary energy, 17 to 20 thicknesses were simulated such that the normalized function,

$$R^* = \left[\frac{R_{FS} - R_{Z_S}}{R_{Z_F} - R_{Z_S}}\right] \qquad (4)$$

is obtained between $0 \leq R^* \leq 1$ . The form of eq.(4) was used by Hunger and Rogaschewski[11] in their study of normalized backscattering coefficient ($\eta^*$) for film-substrate systems. Our attempt to equate their analytic expression of $\eta^*$ to $R^*$ as a simple interpolating formula for $R_{FS}$ have shown limited agreement[6] as the dependence of $R_{FS}$ on the backscattered energy-angular distribution and the ionization cross-section must be accounted for. Barkshire et al.'s[5] assumption in using their analytic formula for unsupported film is valid only for cases when $E_p >> E_b$, i.e. where the ionization cross-section is approximately constant for backscattered energies near $E_P$. It is also valid for cases where the film thickness is relatively thick such that the influence of the substrate is small.

Results of $R^*$ plotted against the normalized mass thickness, s (= $\rho d/\rho d_{0.5}$), for C (KLL) and Al (KLL) for various substrates at 2 to 40 keV were investigated. Substrate influence was reduced implicitly to the normalizing factor $\rho d_{0.5}$, which is the mass thickness for which $R^*$=0.5. The functional form of $\rho d_{0.5}$ can be well described by the expression, C $E_P^m$, as found originally by Holliday and Sternglass[12] from electron range measurements. The range of validity of the function is dependent however on the film ($Z_F$) material, $E_b$ and $E_p$. C and m parameters should in general be dependent on both $Z_F$ and $Z_S$ although they are not significant. Here mean values could be used instead. It is then observed that the normalized behavior of $R_{FS}$, that is for $R^*$, is now to a good approximation dependent only on the film material and primary energy. It can still be described by the functional form as proposed by Hunger and Rogaschewski[11] given by,

$$R^* = \tanh( As + Bs^2 ) \qquad (5)$$

A and B parameters are dependent only on $Z_F$ and $E_P$.

A general equation valid for KLL film-substrate systems will indeed be useful from the results obtained here. At present the LMM/LVV film-substrate systems are also being studied to describe their behavior. With the exponent form derived for $\rho d_{0.5}$ and the input for bulk $R_{Z_F}$ and $R_{Z_S}$ obtained from the fitted expression of Ichimura et al.[13], $R_{FS}$ can then be calculated via eq.(4) and (5) for any thickness s.

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