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# Dependence of the AES backscattering correction factor on the experimental configuration

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ABSTRACT

We present an analysis of the dependence of the backscattering correction factor (BCF) in Auger-electron spectroscopy (AES) on the analyzer acceptance angle. Illustrative BCF calculations are presented for Pd $M_5N_{45}N_{45}$ Auger electrons as a function of primary-electron energy for primary-electron angles of incidence, $\theta_0$, of 0° and 80° and for various values of the analyzer acceptance angle. It was necessary to generalize the BCF definition for the case of an analyzer with an arbitrarily large acceptance angle; this was done with a new function, the integral emission depth distribution function. BCFs calculated from an advanced model of electron transport in the surface region of the Pd sample varied weakly with analyzer half-cone angle for $\theta_0 = 0°$ but more strongly for $\theta_0 = 80°$ where there were BCF differences varying between 19% at a primary energy of 1 keV and 6% at a primary energy of 5 keV. These BCF differences are due in part to variations of the BCF with emission angle and in part to variations of the density of inner-shell ionizations within the information depth for the detected Auger electrons. The latter variations are responsible for differences larger than 10% between BCFs from the widely used simplified BCF model and those from the more accurate advanced model for primary energies less than about 5 keV for $\theta_0 = 80°$. For normal incidence of the primary beam, differences greater than 10% between BCFs from the simplified and advanced models were found for primary energies between 1 keV and 4 keV. These BCF differences indicate that the simplified model can provide only approximate BCF values. In addition, the simplified model does not provide any BCF dependence on Auger-electron emission angle or analyzer acceptance angle.



## 1. Introduction

Auger-electron spectroscopy (AES) is a commonly used technique of surface analysis, particularly in applications that require a high lateral resolution. Four decades ago, Bishop and Riviere [1] proposed a model for quantitative AES in which the Auger signal intensity could be determined from physical properties of the sample and from the analyzer type and configuration. This basic model has been further developed and extended by others [2], and calculated Auger intensities from the extended model have been found to agree substantially with measured Auger intensities for a group of 61 elemental solids [3].

One of the parameters in the latest model for quantitative AES [2,3] is widely known as the backscattering factor (BF). The BF has been defined by ASTM International [4] as the "fractional increase in the Auger current due to backscattered electrons" and by the International Organization for Standardization (ISO) [5] similarly as the "factor defining the increase in the Auger-electron current due to additional ionizations in the sample caused by backscattered electrons above that arising directly from the primary electrons." There are, however, different usages of this term. In some papers, the BF is expressed as the fractional increase and denoted by $r$, while in other papers the BF is expressed as unity plus the fraction increase and is denoted as $R\ (=1+r)$. While the intended BF meaning is generally clear in the context in which it is used, ISO is considering the definitions of two additional terms, the backscattering correction factor (BCF) and the backscattering fraction, that would replace the BF. The proposed definition of the BCF is "factor equal to the ratio of the total Auger-electron current arising from ionizations in the sample caused by both the primary electrons and the backscattered electrons to the Auger-electron current arising directly from the primary electrons." The proposed definition of the backscattering fraction is "ratio of the Auger-electron current arising from ionizations in the sample caused by backscattered electrons and the Auger-electron current arising directly from the primary electrons." Each definition would be accompanied by a common note: "In simple theories, evaluations of the backscattering correction factor or the backscattering fraction may be based on the assumption that the primary beam is unchanged, in intensity, energy or direction, within the information depth for Auger-electron emission. This assumption

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becomes progressively less useful as the primary energy becomes closer to the core-level ionization energy for the relevant Auger transition or for increasing angles of incidence of the primary electrons. In such cases, a more advanced theory of electron transport should be used. For example, if the primary energy is less than twice the core-level ionization energy, the total Auger-electron current emitted from the sample may be less than that calculated for an unaltered primary beam alone so that the effective value of the backscattering fraction is then negative. In addition, the separate classification of electrons as primary or backscattered becomes progressively less useful." In the present work, we utilize the BCF.

Evaluations of the BCF have been made mostly on the basis of a simplified model (as described briefly in the ISO Note). Hall and Morabito [6] pointed out that the BCF is equivalent to the surface-ionization function used in electron-probe microanalysis (EPMA), $\varphi^{EPMA}(z=0)$. The latter function is defined as the surface value of the so-called phi–rho–$z$ function (where $z$ is the depth from the surface) that describes the depth distribution of ionizations in the solid. Hall and Morabito [6] recommended the expression of Reuter [7] for estimating the BCF:

$$R = \varphi^{EPMA}(0) = 1 + 2.8(1-0.9/U_0)\eta, \tag{1}$$

where $U_0$ is the ratio of the primary-electron energy, $E_0$, to the ionization energy, $E_c$, of the core level responsible for the Auger transition of interest, and $\eta$ is the backscattering coefficient, i.e., the probability than an electron of the primary beam will be backscattered with an energy exceeding 50 eV. Jablonski [8] showed in 1980 that the surface-ionization function derived from Monte Carlo simulations by Love et al. [9] compared well with experimental and theoretical BCF values known at that time. The Love et al. expression for $\varphi^{EPMA}(0)$ is:

$$R = \varphi^{EPMA}(0) = 1 + \frac{\eta}{1+\eta}[I(U_0) + G(U_0)\ln(1+\eta)], \tag{2}$$

where

$$I(U_0) = 3.43378 - \frac{10.78720}{U_0} + \frac{10.97628}{U_0^2} - \frac{3.62286}{U_0^3} \tag{3}$$

$$G(U_0) = -0.59299 + \frac{21.55329}{U_0} - \frac{30.55248}{U_0^2} + \frac{9.59218}{U_0^3}. \tag{4}$$

Cazaux [10] proposed a similar expression that additionally took into account the dependence of the BCF on the incidence angle of the primary beam (with respect to the surface normal), $\theta_0$:

$$R = \varphi^{EPMA}(0) \tag{5}$$
$$= 1 + \frac{\eta}{1+\eta}(1+3\cos\theta_0)\left(1-U_0^{-1}\right)\left(1 + \ln\frac{1+\eta}{2}\ln^{-1}U_0\right).$$

The use of Eqs. (1), (2), and (5) requires knowledge of the energies $E_0$ and $E_c$ as well as the backscattering coefficient $\eta$. The latter parameter can be roughly estimated from approximate predictive formulas [7,11].

Shimizu and Ichimura [12–14] performed extensive Monte Carlo calculations of the BCF for numerous solids and for primary energies of 3 keV, 5 keV, 7.5 keV, and 10 keV, energies that were typically used in AES at the time of the calculations. Shimizu analyzed the calculated BCFs and proposed the following simple predictive formulas [14]:

$$R_s = 1 + \left(2.34-2.10Z^{0.14}\right)U_0^{-0.35} + \left(2.58Z^{0.14}-2.98\right)\text{for } \theta_0 = 0^\circ \tag{6a}$$

$$R_s = 1 + \left(0.462-0.777Z^{0.20}\right)U_0^{-0.32} + \left(1.15Z^{0.20}-1.05\right)\text{for } \theta_0 = 30^\circ \tag{6b}$$

$$R_s = 1 + \left(1.21-1.39Z^{0.13}\right)U_0^{-0.33} + \left(1.94Z^{0.13}-1.88\right)\text{for } \theta_0 = 45^\circ \tag{6c}$$

where $Z$ is the atomic number of the solid and the subscript on $R$ denotes Shimizu. These expressions are convenient for use in practical analysis since the BCF is described by a relatively simple function. Of necessity, the formulas are still in widespread use despite the fact that scanning Auger microscopes now routinely operate at primary energies of up to about 25 keV.

Jablonski [15] showed in 2002 that the BCF is defined and evaluated under assumptions that may not be valid in certain analytical situations. It is normally assumed that the primary beam is not changed in intensity, energy, or direction within the information depth for the Auger electrons of interest. In addition, it is assumed that a clear distinction can be made between inner-shell ionizations due to the primary beam and those due to backscattered electrons that enter a thin sample region (defined by the information depth for the detected Auger electrons) from deeper within the solid. These assumptions break down when the primary energy is less than about twice $E_c$ or for near-grazing incidence of the primary beam. In such cases, a more advanced model of electron transport in the solid is required in which the BCF is determined from the excitation depth distribution function (EXDDF) and the emission depth distribution function (EMDDF) [15]. The EXDDF describes the depth distribution of inner-shell ionizations (that can lead to subsequent emission of the relevant Auger electrons) for a specified primary energy and angle of incidence. The EMDDF describes the depth distribution of emitted Auger electrons for a particular emission angle, $\alpha$ (with respect to the surface normal). For an analyzer with a small acceptance angle, the BCF is then given by the simple expression:

$$R^{ADV} = \int_0^\infty \Phi^{NORM}(z, E_0, \theta_0)\phi^{NORM}(\alpha, z)dz, \tag{7}$$

where $\Phi(z,E_0,\theta_0)$ is the EXDDF, $\phi(\alpha,z)$ is the EMDDF, and the superscript on $R$ denotes use of the advanced model. Both functions require a well-defined normalization, as indicated by the superscripts [15]. In several reports, the BCF calculated from Eq. (7) has been found to differ distinctly from values based on the simplified model (i.e., the ASTM and ISO definitions) [15–19].

Calculations of the BCF from the Shimizu predictive formulas [Eqs. (6a)–(6c)] require knowledge of the ratio $U_0$, the atomic number of a solid, and the incidence angle of the primary beam. The use of the advanced definition in BCF calculations [Eq. (7)] requires knowledge of the analyzer position. One should be aware that Eq. (7) has been derived for an analyzer with an infinitely small acceptance angle that is set to accept Auger electrons at the emission angle $\alpha$. In reality, the analyzer acceptance angle must be finite. We note that this acceptance angle can be relatively large for cylindrical-mirror analyzers (CMAs) and the retarding-field analyzers (RFAs) that were often used in early AES equipment. BCFs cannot then be calculated from Eq. (7) for RFAs or for CMAs with their axes at angles other than at right angles to the sample surface.

In the present report, we analyze the dependence of the BCF on the analyzer acceptance angle. The paper is structured as follows. We summarize the relevant theory in Section 2 for calculating the EXDDF, the EMDDF, and then the BCF for an analyzer with its axis set at an arbitrary emission angle and with an arbitrary acceptance angle. In Section 3, we describe Monte Carlo algorithms for BCF calculations based on the simplified and advanced models. We then show calculated BCFs from these two models in Section 4 for the Pd