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Elastic scattering effects in quantitative AES and XPS: Case studies

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Advanced theoretical models of photoelectron and Auger electron transport are typically implemented in Monte Carlo algorithms simulating multiple interactions of signal electrons in a solid. However, much effort has been devoted to develop analytical theoretical models describing electron transport with comparable accuracy. In this review, a critical analysis of these theories is presented. The second issue addressed here is the role of elastic scattering events in quantification of HAXPES analyses performed with the use of polarized radiation.

1. Introduction

Quantitative analysis by electron spectroscopies is based on theoretical models relating the measured AES or XPS signal intensity with the needed characteristics of a solid. Let us tentatively divide procedures to obtain the quantitative information into the following groups: (i) determination of the surface composition; (ii) determination of the overlayer thickness; (iii) estimation of surface sensitivity.

An electron emitted in a solid or backscattered from a solid undergoes multiple elastic and inelastic scattering events. Two theoretical approaches can be used for modeling electron transport in solids: (i) The Monte Carlo simulations of electron transport with different strategies implemented in relevant algorithms, and (ii) advanced analytical models taking into account the multiple interactions of an electron. Furthermore, the theoretical description of photoelectron transport was found to distinctly depend on polarization of X-rays used for sample excitation. Selected issues of the above topics are addressed in the present review.

2. Elastic scattering cross sections

Crucial parameters needed in advanced theoretical models of electron transport are the elastic scattering cross sections: differential, $d\sigma_{el}/d\Omega$, and total, σ_{el}. These values are available from numerous sources. In practical applications, we need the probability density function of scattering angles after one collision, $H_1(\theta)$. A useful source is the series expansion [1]:

$$H_1(\theta) = \frac{1}{\sigma_{el}}\frac{d\sigma_{el}}{d\Omega} = \frac{1}{2\pi}\sum_{l=0}^{\infty}\frac{2l+1}{2l}A_l P_l(\cos\theta) \quad (1)$$

where $P_l(\cos\theta)$ are the Legendre polynomials, and

$$A_l = \frac{2\pi}{\sigma_{el}}\int_0^{\pi}\frac{d\sigma_{el}}{d\Omega}P_l(\cos\theta)\sin\theta\, d\theta \quad (2)$$

These coefficients are generally smooth functions of energy (Fig. 1) which facilitates interpolation. Thus, only an extensive database of coefficients A_l is needed.

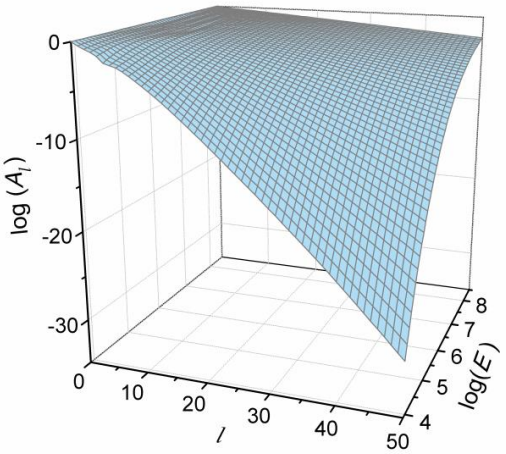

Fig. 1. Energy dependences of the parameters, A_l, for l = 0, 1, 2, …, calculated for tungsten.

3. Determination of the inelastic mean free path for applications in AES and XPS

The inelastic mean free path (IMFP) of electrons is needed in numerous quantitative applications of electron spectroscopies. One of the methods for determination of this parameter is based on measured probabilities of elastic backscattering from surfaces (elastic peak electron spectroscopy – EPES). Relation between the elastic backscattering probability, $d\eta/d\Omega$, and the IMFP, λ_{in}, is expressed with acceptable accuracy by parameters, A_l [1]:

$$\frac{d\eta}{d\Omega} = \frac{\cos\alpha}{\cos\alpha + \cos\theta_0} \sum_{k=1}^{\infty} \frac{s^k}{k} H_k(\theta) \qquad (3)$$

where k is the number of collisions, $s = \lambda_{in}/(\lambda_{in} + \lambda_{el})$, λ_{el} is the elastic mean free path, θ_0 is the electron beam incidence angle, and

$$H_k(\theta) = \frac{1}{2\pi} \sum_{l=0}^{\infty} \frac{2l+1}{2} (A_l)^k \, P_l(\cos\theta) \qquad (4)$$

The code implementing the above formalism was proved to be considerably faster than the typical Monte Carlo approach [2].

4. Surface sensitivity of electron spectroscopies

Surface sensitivity of AES and XPS is conveniently described by the mean escape depth (MED) and the information depth (IF). There are numerous sources of both parameters. An accurate analytical transport theory involving the Chandrasekhar function is a useful source of the MED and the IF [3,4].

In EPES measurements, the surface sensitivity is defined by the mean penetration depth (MPD) of electrons [5]. This parameter is defined as mean depth reached by electrons elastically backscattered from a] solid. The following expression can be derived [5]

$$\mathrm{MPD} = \frac{\lambda_{el} \frac{\cos\alpha}{1+\cos\alpha} \sum_{k=1}^{\infty} s^{k+1} H_k(\cos\theta)}{\sum_{k=1}^{\infty} (s^k/k) H_k(\cos\theta)} \qquad (5)$$

An interesting feature of the dependence of the MPD on the emission angle, α, is the presence of multiple minima and maxima.

5. Determination of surface composition and overlayer thickness.

Elastic scattering effects in AES and XPS can be conveniently accounted for by the use of parameters called the effective attenuation lengths (EAL). In the common formalism of both techniques, the elastic collisions are ignored, and the signal intensity is related to the IMFP, λ_{in}. The EAL parameter is correcting the common formalism for elastic scattering effects when introduced in place of the IMFP. The EALs can be derived from signal intensities obtained from Monte Carlo simulations. However, the analytical transport theories were found to provide numerous parameters with comparable accuracy [3]. The analytical formalism was recently extended to photoelectron energies reaching 5 keV [3] which is of interest for applications of hard X-ray photoelectron spectroscopy (HAXPES). Furthermore, the mathematical form of expressions describing needed parameters can facilitate derivation of the so-called predictive formulas.

The analytical formalism may become rather complicated, and it would be a good practice to publish original computer codes to facilitate applications [2,4].

6. Photoelectrons emitted by linearly polarized synchrotron radiation

It must be stressed here that the typical formalism for excitation by unpolarized X-rays may not apply to experiments performed with the use of polarized radiation. Main reason is due to the fact that the photoelectron intensity depends on the position of the polarization vector. The EMDDF corresponding to a given experimental geometry may considerably differ when the polarization vector is parallel or perpendicular to the surface [6]. As a consequence, the differences are observed in all related parameters. There were attempts to derive the predictive formula for MED and EAL [6], however the dedicated software based on Monte Carlo simulations should be used in general cases, e.g., the NIST Database 100 (SESSA).

7. References

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