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Angle-resolved elastic peak electron spectroscopy: Role of surface excitations

A. Jablonski [a,*], J. Zemek [b]

[a] Institute of Physical Chemistry, Polish Academy of Sciences, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland
[b] Institute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnicka 10, 162 53 Prague 6, Czech Republic

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Abstract

We analyze the possibility of determining the surface excitation parameter (SEP) from the dependence of the elastic backscattering signal intensity on the emission angle. It has been found that the shape of this dependence is reasonably well described by the theoretical model implemented in a typical Monte Carlo simulation strategy. As shown recently, the mean percentage deviation between the experimental angular dependence and the theoretical dependence is equal to 8.82% at 200 eV, 6.28% at 500 eV and 4.69% at 1000 eV. In the theoretical model used, the surface energy losses were ignored. Close inspection of the deviations between theory and experiments indicates systematic trends that can be ascribed to the surface energy losses. We found here that taking into the account the surface energy losses further improves the agreement between theory and experiment. The total mean percentage deviation, equal to 6.65%, decreases to 5.59% if the mathematical form of the Chen formula for SEP is used, or to 5.16% if the Oswald expression is used. The material dependent coefficients in the expression of SEP derived from the emission angle dependence of the elastic peak intensity differ from these coefficients resulting from other methods. We conclude that the determination of SEP from shape of the angular dependence requires the experimental data of high quality, and the reliable theoretical model describing elastic electron backscattering.

Keywords: Computer simulations; Electron–solid interactions; Electron–solid scattering and transmission – elastic; Monte Carlo simulations; Electron spectroscopy; Amorphous surfaces

1. Introduction

Let us consider electrons passing the surface region in solids. Mechanism of inelastic interactions in the surface region may be substantially different from the mechanism of interactions in the bulk. In effect, the number of electrons which survived without energy loss, after passing a certain trajectory and leaving the solid, is different from the number of electrons surviving the same trajectory length traveled entirely in the bulk. Consequently, any theoretical model describing the intensity of signal electrons should take into account the surface energy losses.

In numerous studies, it has been proposed to describe the frequency of the surface energy losses with a surface excitation parameter (SEP) [1–9]. This parameter is defined as the average number of surface excitations during a single surface crossing. In a near future, this parameter may be included into list of parameters important in surface analysis [10]; presently a standardized definition of SEP is being considered.

Surface energy losses decrease the intensity of signal electrons, and the extent of these changes depends on the experimental configuration and the electron energy. For this reason, it would be desirable to account for the surface energy losses in quantification of surface sensitive spectroscopies. However, in analytical practice, the relevant correction typically is not made. This is due to the fact that there is no universal and accurate correction procedure that can be applied to any solid, in particular, the analyzed

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[*] Corresponding author.
E-mail address: ichf@edu.pl (A. Jablonski).

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compound. Furthermore, although a correction for the surface energy losses has a noticeable effect on the signal intensity, the effect is not dramatic in typical experimental configurations. Chen [4] indicated that the shape of the emission angle dependence of the photoelectron signal intensity is not significantly affected for emission angles smaller than about 60°. It has been recently shown that the primary energy dependence of the Au $N_{67}VV$ Auger transition is also not significantly influenced by the surface energy losses [11].

Distinct influence of the surface energy losses is expected in analytical applications of spectroscopies based on measurements of the elastic peak intensity in the energy spectra. The signal electron is passing the surface region twice, entering and leaving the solid. For this reason, the probability of energy losses is increased as compared to photoelectron spectroscopy or Auger electron spectroscopy. The most frequent and useful application of the elastic peak electron spectroscopy is the determination of the inelastic mean free path of electrons in solids [12,13]. It has been demonstrated that the neglect of the surface energy losses may significantly affect the IMFP values [14]. Furthermore, the IMFPs were found to depend on the source for the correction for surface energy losses. Unfortunately, the correction procedure can be made only for limited number of solids for which information on surface energy losses is available.

The SEP parameters can be determined for a particular solid by different methods. Chen [5] published a simple functional representation for SEP with relevant parameters determined for several elements and for GaAs. These parameters were calculated from the dielectric response theory. Werner et al. [6–8] derived the SEP for 16 elements from the REELS spectra. The SEP can also be determined from the energy dependence of the elastic backscattering probability. Tanuma et al. [15,16] measured this dependence using the CMA and also calculated from the Monte Carlo simulations using the IMFP values valid for the bulk of the solid. The difference between measured and calculated elastic backscattering probabilities was ascribed to the surface excitations, which enables the estimation of the SEP. Unfortunately, this approach requires a unique experimental setup making possible absolute measurements of signal electron current entering the analyzer.

Chen [4] indicated that the SEP depends strongly on the emission angle of signal electrons, particularly in the range of glancing emission angles. The calculated angular dependence of photoemission well compares with the experimental data, however, the angular range for this comparison is limited due to experimental restrictions. One can expect that the SEP for elastic peak electron spectroscopy may have pronounced dependence on the emission angle. Consequently, measurements of the angle-resolved elastic peak intensity (AREPES) in wide angular range may provide useful data for determination of the SEP. We address this issue in the present work. In a recent report [17], we have studied the angular distribution of electrons elastically backscattered from different solids. The elastic peak intensities were measured for different solids and energies in a wide range of emission angles. A reasonably good agreement between theory (neglecting the surface energy losses) and experiment has been observed. A question arises if the account for surface energy losses would improve the agreement between theory and experiment. This issue will be a subject of the present paper. Furthermore, we check if the measured emission angle dependences of the elastic peak intensity, on comparison with calculated intensities, would provide a useful method for determination of SEP.

2. Theory

2.1. Expressions describing the SEP

Chen [5] proposed a simple expression for the SEP describing the surface crossing by an electron with energy E at an angle θ with respect to the surface normal:

$$P_s(E,\theta) = \frac{a_{CH}}{E^{1/2}\cos\theta} \tag{1}$$

where a_{CH} is the material dependent parameter. For the model of the free electron gas dielectric function, $a_{CH}^{FEG} = 2.896$ [5].

Werner et al. [6–8] generalized a similar expression, derived earlier by Oswald [18], to the following form:

$$P_s(E,\theta) = \frac{1}{aE^{1/2}\cos\theta + 1} \tag{2}$$

where the parameter a accounts for the material dependence. For the nearly free-electron (NFE) materials, the parameter a is given by [6]

$$a_{NFE} = \sqrt{\frac{8a_0}{\pi^2 e^2}} = 0.1726 \quad (\mathrm{eV}^{-1/2}) \tag{3}$$

Werner et al. [6–8] proposed to describe the surface energy losses with the correction parameter a_W defined by

$$P_s(E,\theta) = \frac{1}{a_W a_{NFE} E^{1/2}\cos\theta + 1} \tag{4}$$

Parameters a_{CH} and a_W reported for different elements are listed in Tables 1 and 2.

Table 1
Comparison of the coefficients a_{CH} (Eq. (1)) published by Chen [5] with coefficients determined in the present work

Element	Present work	Chen [5]
Silicon	2.996	2.50
Iron	3.087	2.51
Cobalt	0.871	–
Nickel	1.189	–
Copper	5.295	2.45
Palladium	0.386	–
Silver	0.585	2.34
Samarium	0.775	–
Iridium	1.676	–
Gold	4.185	3.06