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Energy dependence of electron energy loss processes in Ge 2s photoemission

M. Novák [a,*], S. Egri [b], L. Kövér [a], I. Cserny [a], W. Drube [c], W.S.M. Werner [d]

[a] Institute of Nuclear Research of the Hungarian Academy of Sciences (MTA ATOMKI), 18/c Bem tér, H-4026 Debrecen, Hungary
[b] Department of Experimental Physics, University of Debrecen, 18/a Bem tér, H-4026 Debrecen, Hungary
[c] Hamburger Synchrotronstrahlungslabor am Deutschen Elektronen-Synchrotron DESY, Notkestr. 85, D-22603 Hamburg, Germany
[d] Institut für Allgemeine Physik, University of Technology, Wieder Hauptstrasse 8-10, A 1040 Vienna, Austria

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Abstract

Deep core Ge 2s photoelectron spectra from polycrystalline Ge films induced by monochromatic synchrotron radiation, of 4, 6 and 8 keV were measured and analysed using two different methods, the partial intensity analysis and the extended Hüfner method to determine the spectral contributions from different electron energy loss processes due to bulk extrinsic, intrinsic and surface excitations. The obtained photon energy dependence of the ratio of these contributions was compared as a function of the photoelectron kinetic energy. It was found that the relative contribution of intrinsic excitations increase with the photon energy.

Keywords: X-ray photoelectron spectra; Intrinsic loss; Extrinsic loss; Surface excitation

1. Introduction

Energy loss processes for electrons excited by X-rays from solids are of crucial importance for a quantitative interpretation of XPS and photoinduced Auger spectra. For the accurate quantitative analysis of the measured spectra the contributions from the different energy loss processes within 100 eV below the photoelectron peak should be known, because these characteristic effects also appear in the energy region influencing the peak shape. The electron energy loss processes, which have considerable effect on the shape of the measured spectra are: bulk extrinsic excitations (due to inelastic interactions of photoelectrons during their transport within the bulk solid), bulk intrinsic excitations (due to the sudden creation of the core hole and its screening by electrons in the solid environment) and surface related excitations (as a consequence of surface crossing of the emitted electrons) and also electron–hole pair creation. The separation of the contributions from the different loss processes is important in order to disentangle the primary intrinsic spectrum and its modification caused by the electron transport as well as to understand the nature of these processes by applying sophisticated evaluation methods [1,2]. Such information is especially relevant for high energy X-ray induced electron spectroscopy which is gaining importance in the analysis of deeply buried interfaces. In this work, Ge 2s ($E_B = 1415$ eV) photoelectron spectra induced by synchrotron radiation at different photon energies are presented and analysed using two different methods to determine contributions attributable to different electron energy loss processes. The photon energy dependence of the ratio of these contributions is derived and discussed.

2. Experimental

Ge layers of 100 nm thickness were vacuum deposited onto Si wafer substrates using a D.C. magnetron and

* Corresponding author.
E-mail address: M.Novak@atomki.hu (M. Novák).

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cleaned in situ by Ar ion sputtering prior to the measurement. Ge 2s photoelectron spectra were measured using the tunable high energy XPS facility at the BW2 beamline of HASYLAB at DESY (Hamburg). Photon energies of 4 keV, 6 keV and 8 keV were chosen for this experiment. The incidence photon beam was 45° while the angle of analysed beam was 0° with respect to the surface normal of the sample. Further experimental details can be found in Ref. [3].

3. Methods of data analysis

3.1. Partial intensity analysis

At the high excitation energies used in this experiment, the sudden approximation is fulfilled (also in the case of the Ge 2s photoemission) and the classical three step model (photoionisation, electron transport and emission) of the photoelectron emission from solids can be applied. Within this model the shape of the primary excitation spectrum is modified mainly by the energy loss processes mentioned above. The measured photoelectron energy distribution $Y(E)$ is a superposition of these contributions [1]

$$Y(E) = \sum_{n_1=0}^{\infty}\sum_{n_2=0}^{\infty}\sum_{n_3=0}^{\infty}\cdots C_{n_1n_2n_3\ldots} f_0(E) \otimes L_{n_1n_2n_3\ldots}(E) \tag{1}$$

where $C_{n_in_jn_k\ldots}$ are the partial intensities which represent the number of the electrons participating n_i times in the i type loss process and n_j times in the j type loss process etc., f_0 denotes the primary energy distribution of the photoinduced electrons (source function) without distortions due to electron transport and $L_{n_i\ldots}(E)$ represent the probability distribution of the electrons losing energy participating n_i times in i type energy loss process. The symbol "$\otimes$" denotes a convolution over the energy variable.

The partial intensity analysis method [1] is based on the assumption that the loss processes are uncorrelated, independent processes which is a good approximation in many cases. Then

$$L_{n_1n_2n_3\ldots}(T) = L_{n_1}(T) \otimes L_{n_2}(T) \otimes L_{n_3}(T) \otimes \cdots \tag{2}$$

$$C_{n_1n_2n_3\ldots} = C_{n_1}C_{n_2}C_{n_3}\ldots \tag{3}$$

The contribution of a particular loss process from the measured spectrum can be removed by the iterative correction procedure

$$Y_{k+1} = Y_k(E) - q_k \int Y_k(E+T)L_k(T)\mathrm{d}T \tag{4}$$

where Y_0 is the measured spectrum, L_k is the probability distribution of the energy loss of the electrons after participating in k times in the given loss process. q_k is the function of the normalised partial intensities [1].

The bulk extrinsic excitations are described by the differential inverse inelastic mean free path (DIIMFP) $W_\mathrm{b}(T,E)$, which is related to the dielectric function of the medium $\varepsilon(q,T)$ [1].

$$W_\mathrm{b}(T,E) = \frac{1}{\pi a_0 E}\int_{-q}^{+q}\frac{\mathrm{d}q}{q}\,\mathrm{Im}\left(\frac{-1}{\varepsilon(q,T)}\right) \tag{5}$$

The normalised DIIMFP is the probability distribution of the energy loss in one bulk extrinsic excitation (L_1).

The partial intensities for the bulk extrinsic process were calculated by Monte Carlo simulation [4] taking into account both elastic and inelastic scattering of the electrons.

The distribution of energy losses for an electron crossing the solid–vacuum interface is determined by the surface energy loss function $\mathrm{Im}\left(\frac{-1}{\varepsilon(q,T)+1}\right)$ instead of the bulk energy loss function $\mathrm{Im}\left(\frac{-1}{\varepsilon(q,T)}\right)$.

For partial intensities concerning surface losses we assume

$$C_{n_\mathrm{s}} = \langle n_\mathrm{s}\rangle^{n_\mathrm{s}}\exp(-\langle n_\mathrm{s}\rangle)/n_\mathrm{s}! \tag{6}$$

where $\langle n_\mathrm{s}\rangle$ denotes the average number of surface excitation in a single surface crossing (surface excitation parameter, SEP) [5,6].

Furthermore, it is assumed that intrinsic excitations have the same energy loss distribution as bulk extrinsic excitations [7] and the normalised partial intensities for multiple intrinsic excitations also follow an equation of the type (6), so that the reduced partial intensities are given by

$$c_{n_\mathrm{intr}} = b^{n_\mathrm{intr}}/n_\mathrm{intr}! \tag{7}$$

where the parameter b is the intrinsic creation rate with typical values between 0.1 and 0.6.

3.2. Extended Hüfner model

We have developed a simple method to analyse the energy loss part of photoinduced electron spectra and separate contributions from different type of losses. It is an extension of the method originally proposed by Steiner et al. [8]. The new model – compared to the original one – applies more realistic functions for describing energy loss distributions of single inelastic interactions, accounts correctly for multiple losses of different origin and includes surface contributions [9]. The model photoelectron spectrum using this extended model can be written as [9]

$$\begin{aligned} Y_\mathrm{model} = {} & A_0 + A_0 \otimes L_\mathrm{b} b + A_0 \otimes L_\mathrm{b} a \\ & + \sum_{n=2}^{\infty} A_0 \otimes L_\mathrm{b}^{n-1}\left(\frac{b^n}{n!} + \sum_{i=1}^{n-1} a^i \frac{b^{(n-i)}}{(n-i)!} + a^n\right) \\ & + \sum_{z=1}^{\infty} A_0 \otimes L_\mathrm{s}^{(z-1)}\frac{c^z}{z!} + \sum_{n=1}^{\infty}\sum_{z=1}^{\infty} A_n \otimes L_\mathrm{s}^{(z-1)}\frac{c^z}{z!} + B \end{aligned} \tag{8}$$

where Y_model is the resulting model function, A_0 is the photopeak, approximated by a Doniach–Sunjic (DS) function convoluted with the spectrometer response function of a normalised Gaussian shape. L_b and L_s are the normalised DIIMFP and normalised DSEP, respectively, calculated from optical data, n is the order of the bulk plasmon