Ni és Ge felületi rétegekből keltett K-Auger spektrumok elemzése

Analysis of K-Auger spectra excited from surface layers of Ni and Ge

doktori (PhD) értekezés tézisei

abstracts of Ph.D. thesis

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Introduction

Photon induced electron spectroscopy is a powerful tool for the investigation of the surface and the electronic structure of matter. Electrons analyzed by the widely used methods (X-ray Photoelectron Spectroscopy, X-ray Auger Electron Spectroscopy) applying low energy (0,5 – 2 keV) photons for excitation of the spectra are originated from the several nm thin surface region. Due to the latest developments in technology, applying higher excitation energies (2 -10 keV) and the precise analysis of electrons within high kinetic energy become available. As a consequence increasing number of experimental works using high energy photons for excitation of the core electrons of heavy elements are published.

Throw these high energy methods the possibilities of electron spectroscopy becomes wider. Using them, the effect of the surface becomes less important, while the information depth increases up to 20-30nm, witch allows to investigate deeply buried layers in a non-destructive way, unfortunately with decreasing energy resolution. Besides the applications in surface analysis, high energy methods require and support the understanding of the underlying physical processes, concerning with the ionization of the core shells, and gave a unique possibility to verify the applicability of the quantum mechanical models for describing the Auger and photoelectron process and the solid as well.

In order to extract useful information about the composition and the chemical state of the components from the measured high energy Auger and photoelectron spectra we should take into account the effect of the transport of the emitted electrons along they path throw the solid, the effects of multiple elastic and inelastic collisions. The scattering properties of the matter can be evaluated from the electron energy loss, or reflected electron energy loss spectra (EELS, REELS). In these methods the electrons penetrated into the matter and suffered several inelastic collisions are investigated.

Measured spectral shape reflects the physical properties of the Auger transition, and effects of secunder processes, taking place along with the Auger transition. The evaluation of K-Auger spectra can reveal the nature of these processes.

In order to interpret the measured Auger transition energies the correlation of the two holes appearing in the final state of the transition should taken into account. From the theoretical point of wiev the handling of the correlation between the two holes of the final state and the way of taking account the screening of the charge of the atomic nucleus are important questions. Moreover, throw evaluation of the spectra final and initial state shake processes in conjunction with the photo ionization of the core shell, the effect of the local density of states (LDOS) to the spectral shape, the Coster Kronig transitions and Auger cascade processes can be investigated.

Studied problems and applied methods

High energy electron spectra excited from polycrystalline Ni and Ge were studied.

At first, reflection electron energy loss spectra (REELS) were investigated for 200eV-5keV electrons backscattered from Ge surfaces. Effects of multiple bulk elastic and inelastic scattering was eliminated from the measured spectra using precise collision statistics calculated with the Monte Carlo simulation of the respected electron tajectories. The total surface excitation probability (SEP) was derived. A material parameter was derived from the measurements that describe the dependence of the average number of surface excitations experienced in a single surface crossing on the electron energy and direction of the surface crossing by using modified formulae of Oswald. This parameter was used in further evaluation of measured Ge photoelectron and Auger spectra.

2s photoelectron spectra of polycrystalline Ge film excited with high energy synchrotron radiation were studied. Effects of the multiple bulk inelastic and elastic scattering, multiple inelastic scatterings near the surface and intrinsic collective excitation of the valence electrons due to the appearance of the inner shell vacancy were eliminated from the measured spectrum by Partial Intensity Analysis. The asymmetry of the remained peak is similar to Donijah-Sunjic line-shape and attributable to the effect of the electron-hole pair creations. In this work these results are shown as an illustration of the usage of Partial Intensity Analysis.

Ge $KL_{23}L_{23}$ Auger spectra photoexcited (using bremsstrahlung radiation) from thin Ge films were measured with high energy resolution. The measured spectra were corrected for effects of inelastic scattering within the films using Partial Intensity Analysis and using Tougaard-type background correction as well. Effects of the collective intrinsic excitations of the valence electrons were taken into account by using complex peak shapes were generated from asymmetric Lorentz functions. The relative transition energies, the absolute transition energy of the most intense Auger line, the relative intensities and the energy widths of the $KL_{23}L_{23}$ Auger lines were evaluated from the measured spectra.

The X-ray excited KLM Auger spectrum of a 2 micrometer thick nickel film was measured with high energy resolution excited by tunable monochromatizes synchrotron radiation with 9,2keV. The measured spectra were corrected for effects of inelastic scattering inside the sample by using Partial Intensity Analysis method, effects of collective intrinsic type excitation of valence electrons were taken into account by using complex peak shapes were constructed from asymmetric Lorentz functions. The relative Auger transition energies, the absolute transition energy of the most intense Auger line, the relative intensities and the energy widths of the KLM Auger lines were evaluated from the measured spectra. Effects of multiplett splitting due to the intermediate coupling model of the angular momenta and presence of the photoelectron peaks excited by the characteristic X-rays photoinduced internally in the sample was also taken into account during the evaluation.

New scientific results

Surface excitation parameter of Ge

Reflection electron energy loss spectra (REELS) was measured for 500, 1000, 2000, 5000 eV electrons backscattered from the surface of 200 nm thick polycrystalline Ge film with high energy resolution. (0.4 -0.6 eV) The average number of the surface plasmons excited by the backscattered and detected electrons during the surface crossing (integral Surface Excitation Parameter) and the respective only material dependent parameter was derived from the spectra by using the method Partial Intensity Analisys. For modelling the electron scattering within the sample electron trajectories were simulated by Monte Carlo simulation.[1]

$KL_{23}L_{23}$Auger electron spectrum of Ge

(a)

Transition energies of Ge $KL_{23}L_{23}$ Auger lines was evaluated from the measured spectra excited from the 100 nm thick polycrystalline Ge film by high energy photons. Results were compared with experimental results evaluated from spectra excited by electrons from thin film in transmission geometry and from spectra from radioactive sample. The relative energies are in good general agreement with previously published ones and also with the results of the theoretical calculations. The absolute energy of the most intense $^1D_2$ line is in very good agreement with the result of radioactive experiment, which means, that the different way of excitation do not causes significant difference in the energies of the respected Auger transitions. [2]

(b)

The measured relative energy of the strong satellite originated from intrinsic loss process on the low energy tail of the intense $^1D_2$ line differs significantly (by 4 eV) from the results of previous measurements. Possible cause of this deviation is that the background correction procedure was used in the previous work based on the energy loss distribution derived from loss spectrum of electrons passing throw the 10 nm thin sample which loss spectrum contained contribution from surface and multiple bulk loss processes. Because of this, the intensity of the $^1S_0$ peak and the plasmon peak was partly removed by the background correction which caused the 4 eV shift in the energy position of the plasmon. [2]

(c)

Relative transition intensities to the most intense $^1D_2$ line derived from the background corrected spectra are in good agreement with the respective results evaluated from the spectra originated from radioactive sample on contrary, there are major deviations from the results of the evaluation of the experiment using electron excitation and 10 nm thin film in transmission geometry. The overestimation of the relative intensity of the KL_3L_3 ($^3P_0$) line attributable to the neglection of the intrinsic energy loss tail of the $^3P_2$ line, the underestimation of the relative intensity of the KL_2L_2 ($^1S_0$) line, as well as the much smaller plasmon peak intensity are caused by the inaccuracy of the applied background correction procedure due to the contribution of the surface and multiple bulk inelastic scattering to the applied energy loss spectrum. Taking into account these effects in two alternative ways, my results are in good agreement with the respective Auger intensities obtained from relativistic atomic calculations and in the intermediate coupling scheme. [2]

KLM Auger spectrum of nickel

(a)

Relative energies of the identified Auger diagram lines to KL_2M_{23} $^1D_2$ peak were evaluated from the Ni KLM Auger spectra measured at the first time. Derived relative energies are in good overall agreement with relativistic calculation on the basis of intermediate coupling model. Higher deviations occurred in the cases when unclosed M_{45} subshell was participated in the transition. In contrary to previous works due to the better energy resolution and statistics instead of nine peaks we used 13 peaks for fitting the background corrected spectrum. The appearance of extra peaks can be explained as a consequence of the applicability of the intermediate coupling model for describing the electron correlation in the final state of the Auger transition, and as a consequence of the photo excitation of 3s and 3p electrons by the characteristic $K\alpha_1$ radiation of nickel, originated from the radiative relaxation of the vacancy in the K-shell. [3]

(b)

Intensities of the Auger diagram lines related to the most intense KL_2M_{23} $^1D_2$ peak were evaluated from the spectra, with a good agreement with relativistic calculations using intermediate coupling scheme, even in the case of KL_3M_{23} line, while theoretical calculations using jj-coupling scheme gives nearly two times higher relative intensity for this line. Measured results follow the trends of previous measurements on transition metals Z=23-26, excited by photons and originated from radioactive sample.[3]

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