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Fine structure of inelastic electron scattering cross-section spectra for MN

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Abstract. The comparative analysis of the reflection electron energy loss spectra and the inelastic electron scattering cross-section spectra for Mn was carried out. It is shown that inelastic electron scattering cross-section spectra have certain advantages in the study of the interaction of electrons with the substance as compared to the electron energy loss spectra. The inelastic electron scattering cross section spectra fine structure was analysed by fitting the experimental spectra using the 3 parameters Lorentzian-type formula of Tougaard. This method was used for the quantitative analysis of the contributions of various loss processes in the inelastic electron scattering cross section spectra, determination of the loss peaks energies and origin.

1. Introduction

Mn is widely used in multilayer metal/semiconductor structures, which open opportunities for the development of micro-, nanoelectronics and spintronics [1, 2]. The study of multilayer structures physics, metal/semiconductor interfaces and silicidation processes are necessary for the development of nanotechnology. One of the most informative methods of research materials is electron spectroscopy, in particular reflection electron energy loss spectroscopy (REELS). From REEL spectra the inelastic electron scattering cross section spectra (so-called $K\lambda$-spectra [3]) can be calculated and allow to investigate the electron-solid inelastic interaction more detailed [2, 4-10]. Analysis and interpretation of the electronic spectra are important for understanding the physical processes of the investigating systems. Both the REELS and $K\lambda$-spectra for Mn are underinvestigated.

Inelastic electron scattering cross section spectra indicate the probability of electron energy loss T in a single scattering event. $K\lambda$-spectra can be used for quantitative determination of element concentrations in two-component composite structures. The ability of quantitative

determination of atomic element concentrations in Fe_xSi_{1-x} [5, 6], Mn_xSi_{1-x} [2] and Ge_xSi_{1-x} [7] systems were investigated earlier with the dependence of the maximum value of $K\lambda$-spectra for the standard samples. Computer modeling of inelastic electron scattering cross section spectra in terms of the dielectric response theory was used for the investigation of elements depth distribution and for determination of silicon dioxide film thickness on a silicon substrate [6].

In this paper, the method of fine structure analysis of inelastic electron scattering cross-section spectra suggested by us in [9, 10] is applied to analysis of Mn $K\lambda$-spectra. This method is based on fitting inelastic electron scattering cross-section spectra to the 3 parameters Lorentzian-type formula of Tougaard [11] and used for determination the origin of the loss peaks and unresolved peaks analysis.

2. Experimental

The spectra for Mn were measured employing two multilayer systems composed of (1) Si substrate, 50 nm Mn film, 30 Å Pd layer protecting the Mn layer from oxidation and (2) glass substrate, 50 nm Mn film, and protecting 30 Å Ge layer. The samples were prepared using the thermal evaporation method under high vacuum conditions.

The experiments were carried out using a photoelectron spectrometer SPECS (Germany) equipped with the spherical energy analyzer PHOIBOS MCD9, double anode X-ray tube as an X-ray source, and a Microfocus EK-12-M electron gun (STAIB Instruments) for excitation of the REEL spectra. The surface contaminations, protecting layers and oxide layers were removed applying Ar^+ ion etching (accelerating voltage of 2.5 kV, ion current of 15 μA) with an ion source IQE-12/38 (SPECS) in the analytical chamber of the spectrometer before the REELS measurements; the completeness of the procedure was controlled via the relevant photoelectron and Auger spectra.

REEL spectra were acquired in the interval of 150 eV below the elastic peak with an energy step of 0.1 eV. Energy loss T was calculated as the difference between the primary electron beam energy E_0 (zero loss) and the reflected electron energy E, $T = E_0 - E$. The primary electron beam energies were 300, 600, 1200, 1900, 3000 eV, and the full width at half-maximum (FWHM) of the primary electron beam was less than 1 eV.

The inelastic electron scattering cross section spectra which are the products of inelastic mean free path λ and inelastic scattering cross section $K(E_0, T)$ (where E_0 is the primary electron energy, $T = E_0 - E$ is the electron energy loss and E is the reflected electron energy) were calculated from the experimental reflection electron energy loss spectra with the software package QUASES™ XS REELS (Quantitative Analysis of Surfaces by Electron Spectroscopy cross section determined by REELS) [12] based to the algorithm suggested in [13].

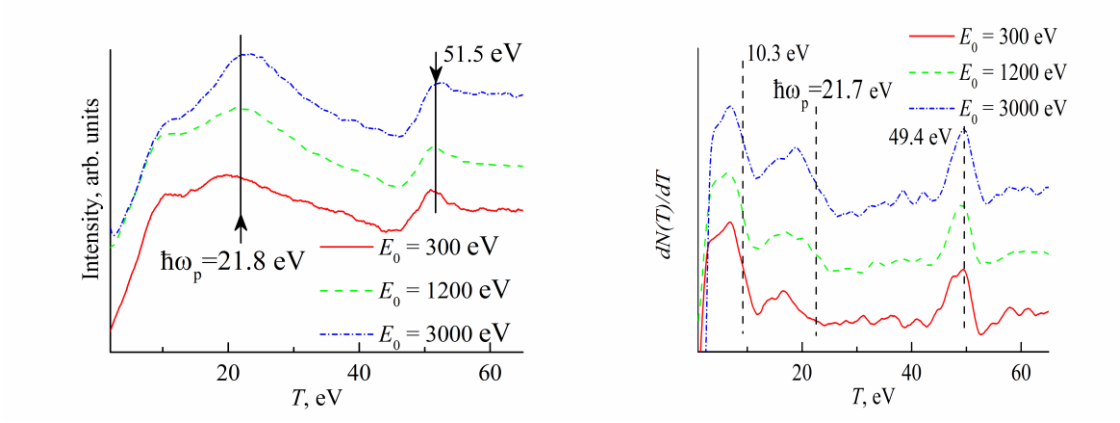
3. Results and discussion

3.1. The comparative analysis of the reflection electron energy loss spectra and the inelastic electron scattering cross-section spectra for Mn

On the REELS for Mn (Fig. 1, a) there are two peaks: the intensive peak at energy 21.8 eV and less intense one at energy 51.5 eV, corresponding respectively to excitations of volume plasmon and core level excitation M_{23} in Mn. In the low-energy region the feature with energy of about 5 eV is observed.

For the more accurate peak energy determination and reducing of the impact of inelastic electrons background, numerical differentiation of the experimental curves $N(T)$ (N is the

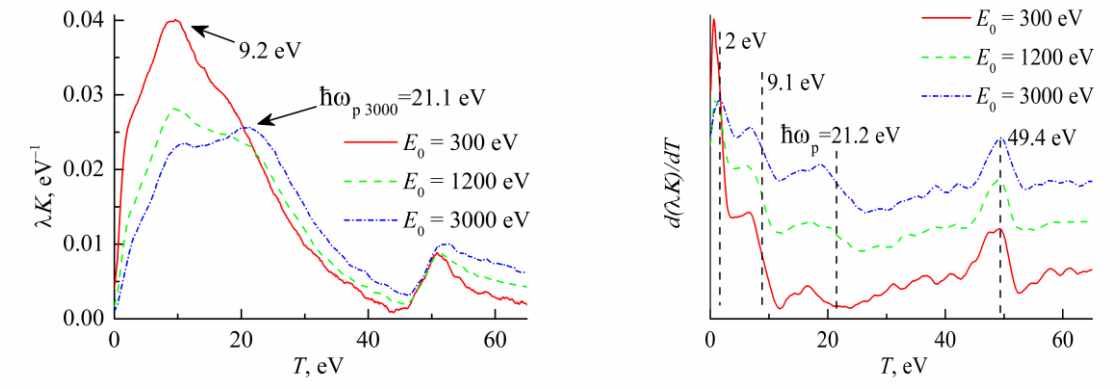
number of electrons with energy loss T) was carried out (Fig. 1, b). In the differential spectra for Mn in addition to the bulk plasmon and M_{23} peak, the peak at energy 9 eV is observed. The average loss peaks energies determined from the differential REELS are 10.3 ± 1.0, 21.7 ± 1.4 and 49.4 ± 0.2 eV. The surface plasmon is not resolved in these spectra. Peak energies are close to the literature data for manganese [2, 14-16].



a) b)

Figure 1. Reflection electron energy loss spectra for Mn in integrated (a) and differential (b) species.

The inelastic electron scattering cross-section spectra for Mn obtained with primary electron energies 300, 1200, 3000 eV are shown in figure 2.



a) b)

Figure 2. Inelastic electron scattering cross-section spectra for Mn in integrated (a) and differential (b) species.

Inelastic electron scattering cross-section spectra in contrast to REELS have absolute units of energy loss. At figure 2 (a) the variation of spectrum shape with primary electron energy is observed: at E_0 = 300 eV the peak at 9.2 eV is dominating and it decreases with E_0. At E_0 = 3000 eV the peak at 21.1 eV, corresponding to volume plasmon loss in Mn [2, 14, 15], is dominating. It is worth noting, that the $K\lambda$-spectrum shape is more affected by the variation of primary electron energy that the REEL spectra. This is probably generated by the increasing of surface loss intensity in consequence of the subtraction of multiple electron scattering background according to algorithm [13]. At these spectra the M_{23} peak is always observed. At figure 2 (b) the differential $K\lambda$-spectra for Mn is shown. Differentiation allows us to determine

the energy of low-intensity peak at 2 eV, but surface plasmon is still not resolved. The average loss peaks energies determined from the differential $K\lambda$-spectra are 2.0 ± 0.5, 9.1 ± 0.2, 21.2 ± 1.8 and 49.4 ± 0.2 eV. These energies are closed to loss peaks energies obtained from REELS.

3.2. The fine structure of inelastic electron scattering cross-section spectra analysis

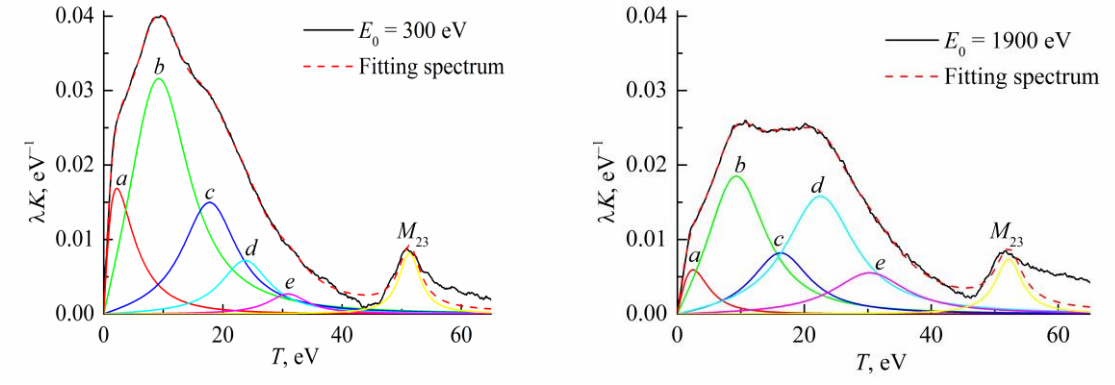
The variation of inelastic electron scattering cross section spectrum shape with the primary electron energy is affected by the variation of surface-like and volume-like excitation intensities. In Ref. [9, 10] the method of inelastic electron scattering cross-section spectra fine structure analysis was suggested. The fine structure analysis is based on fitting $K\lambda$-spectra to the 3 parameters Lorentzian-type formula of Tougaard [11]:

$$\lambda K = \frac{BT}{\left(C - T^2\right)^2 + DT^2}.$$

B, C, D are fitting parameters and have special values for different elements [11]. The peak intensity depends on parameter *B*, peak energy depends on parameter *C*, peak width and, indirectly, peak energy depend on parameter *D*.

We chose the 3 parameters Lorentzian-type formula of Tougaard because it describes the inelastic electron scattering mechanisms. The $K\lambda$-spectra fitting to the Tougaard peaks can be used to analyze different mechanisms of inelastic electron scattering such as volume plasmon excitations, surface plasmon excitations and interband transitions.

The results of fitting the Mn $K\lambda$-spectra that were obtained with primary electron energies 300 and 1900 eV is shown in figure 3.



a) b)

Figure 3. The inelastic electron scattering cross-section spectra for Mn obtained with primary electron energies 300 (a) and 1900 (b) eV fitted to the 3 parameters Lorentzian-type formula of Tougaard.

The number of fitting peaks was chosen to provide the minimal least-square deviation of the fitted spectrum from the experimental spectrum. Six peaks including peak M_{23} are sufficient to provide a good coincidence between the experimental and fitting spectra. The inelastic electron scattering cross-section spectra for Mn were approximated with 6 Tougaard peaks *a, b, c, d, e* and peak M_{23} (core level excitation [2, 14, 16]). Parameters *B, C, D* of the 3

parameters Lorentzian-type formula of Tougaard were varied for the best least squared fit to the experimental spectra.

The primary energy dependences of the fitted peak areas (that describes the excitation intensity) are shown in figure 4. The gradual decrease with primary energy areas of peaks *b* and *c* indicate their surface origin (surface-like peaks); the opposite primary energy dependence of the peak *d* area indicates its bulk origin (volume-like peak). The other peaks origin is hard to determine because of their small intensity.

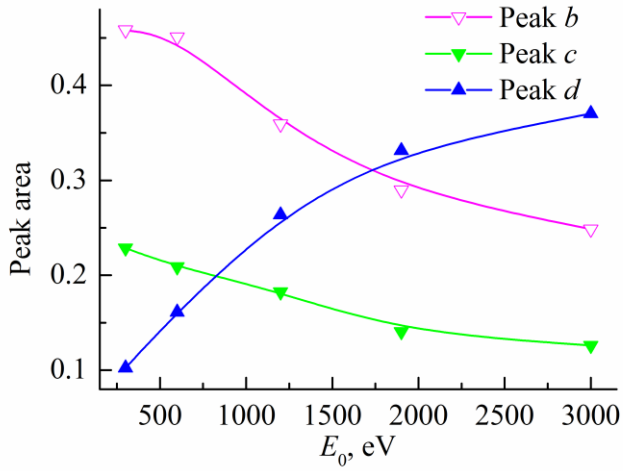


Figure 4. The primary energy dependences of the fitting peaks area

The average energies of the fitted peaks and their root-mean-square deviation are shown in Table 1. The fine structure analysis method allows determining the peaks energies balancing out an effect of summation of different losses intensities to the energies of spectrum maximums.

Table 1. Fitting peaks energies

Fitting peak	*a*	*b*	*c*	*d*	*e*	M_{23}
Fitting peak energy, eV	2.5 ± 0.4	9.2 ± 0.1	16.9 ± 0.8	23.0 ± 0.6	30.6 ± 0.6	51.8 ± 0.4

The volume-like peak *d* corresponds to volume plasmon because it has gradually increasing primary energy dependence of area and its energy loss is close to the bulk plasmon energy in Ref. [2, 14, 15] (Table 1). Peak *c*, corresponds to a surface plasmon because it has gradually decreasing primary energy dependences of area and the energy loss ratio between the volume plasmon and the peak *c* is 1.35 that is quite close to the well-known $\sqrt{2}$ from the classical plasmon model [15, 17]. This peak was unresolved in REELS and $K\lambda$-spectra for Mn but the method of fine structure analysis allows determining its energy, intensity and origin. The M_{23} peak related to the electron transition from the level M_{23} and its energy loss is close to the literary data for Mn [2, 14, 16].

This method is look like the method of fitting the XPS spectra to the peaks. The functions used in XPS-spectra fitting are Gaussian-Lorentzian curves (Voigt-functions) and Doiach-Sunjic functions [18]. The peak fitting in spite of some difficulties with mathematical uncertainty became an important tool in XPS [18, 19] that is used for the chemical binding determination. The peak fitting in inelastic electron scattering cross section spectroscopy can be used for the investigation of electron scattering mechanisms and quantitative determination of the different processes contributions to the inelastic electron scattering cross section spectra.

4. Conclusions

The reflection electron energy loss spectra and the inelastic electron scattering cross-section spectra for Mn were investigated. Comparative analysis of these spectra shown, that the inelastic electron scattering cross-section spectra are more sensitive to changes in the primary electron energy and allow to analyze, not only energy, but also the intensity of the losses. To investigate the fine structure for Mn inelastic electron scattering cross-section spectra the method based on its approximation with 3 parameters Lorentzian-type formula of Tougaard was applied. Using the fine structure analysis method the investigation of the unresolved loss peaks, determination of its energies and origin were carried out.

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