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Electron scattering in matter taking into account surface effects

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Abstract. This paper presents a model of inelastic electron scattering in a substance, taking into account surface effects. The surface effects were taken into account when calculating the differential cross sections of inelastic scattering based on the dielectric theory of Drude. In this paper, the transmission function was calculated when solving the transfer equation using two methods: the matrix method and the Monte Carlo method. Based on the transmission functions obtained, the energy spectra of X-ray photoelectron spectroscopy (XPS) were calculated. Computational and simulation models of inelastic electron scattering in matter have been proposed to implement methods for solving the transport equation.

Keywords: electron spectroscopy, inelastic scattering, surface effects, transmission function, Monte Carlo method

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Рассеяние электронов с учетом поверхностных эффектов

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Аннотация. В данной работе представлена модель неупругого рассеяния электронов в веществе с учетом поверхностных эффектов. Поверхностные эффекты были учтены при расчете дифференциальных сечений неупругого рассеяния на основе диэлектрической теории Друде. В работе была посчитана функция пропускания при решении уравнения переноса двумя методами: матричным методом и методом Монте-Карло. На основе полученных функций пропускания были посчитаны энергетические спектры рентгеновской фотоэлектронной спектроскопии (РФЭС). Для реализации методов решения уравнения переноса были предложены расчетная и имитационная модели неупругого рассеяния электрона в веществе.

Ключевые слова: электронная спектроскопия, неупругое рассеяние, поверхностные эффекты, функция пропускания, метод Монте-Карло

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Introduction

The problem of an adequate description of the energy losses of high-energy electrons passing through a layer of matter is of interest. This problem often concerns such fields as nano- and microelectronics, physics of nanostructures, metal science, etc.

The transmission function is the basic function of any electron spectroscopy, the physical meaning of which is the distribution function of electrons passing through a layer of matter according to the energy they lost as a result of inelastic scattering. This function was first obtained by L.D. Landau [1]. The results obtained in this work only qualitatively describe experimental data, the accuracy of Landau's solution is very low, this is primarily due to the fact that at that time the behavior of the differential cross section of inelastic scattering in the region of low energy losses was not known. Much later, in [2], Landau's solution was modified by using the threshold cross section of inelastic scattering, and in this work, the invariant immersion method derived a formula for the transmission function over scattering multiplicities, which describes the experiment better than Landau's solution.

The work [3] was one of the first in which surface effects were taken into account when calculating the transmission function. The idea was to represent the layer in the form of surface and bulk layers. The disadvantage of these methods is that some parameters are adjustable. However, there is another way. In [4–5], Differential Inverse Inelastic Mean Free Path (DIIMFP) are derived based on the dielectric theory of Drude, which depend on the scattering coordinate, the angle of entry (departure) of the electron, and the energy of the electron. Based on these DIIMFP, the surface effects on electron scattering in matter will be taken into account in this work.

Materials and methods

We can find the transmission function if we solve the transfer equation:

$$\frac{dT_{in}(z,\Delta)}{dz} = \lambda_{in}^{-1}(z)\cdot\left[-T_{in}(z,\Delta)+\int_0^{\Delta} T_{in}(z,\varepsilon)X_{in}(z,\Delta-\varepsilon)d\varepsilon\right], \qquad (1)$$
$$T_{in}(0,\Delta)=\delta(\Delta),$$

where $T_{in}(z, \Delta)$ is the transmission function, λ_{in} is the Inelastic Mean Free Path (IMFP), $X_{in}(z, \Delta)$ is the unit-normalized differential cross section of inelastic scattering, z is the coordinate of the scattering point, Δ is the energy loss.

Equation (1) can be solved using two methods: the matrix method and the Monte Carlo method. The matrix method is implemented if we represent the convolution in equation (1) as a product of matrices. When substituting matrices into the transfer equation, a matrix-vector equation is obtained, which is solved by methods of the theory of differential equations:

$$\mathbf{T}(z,\Delta)=\operatorname{expm}\left[-\int_0^d \lambda_{in}^{-1}(z)\left(\mathbf{E}-\mathbf{A}(z)\right)dz\right]\mathbf{D}, \qquad (2)$$

where $\mathbf{E}$ is the identity matrix, $\mathbf{A}(z)$ is the Toeplitz matrix, which is necessary for calculating the convolution, $\mathbf{D}$ is the matrix equivalent of the Dirac function, expm ( ) is the matrix exponential function.

To implement the Monte Carlo method, it is necessary to create a simulation model of inelastic electron scattering in matter, and then use this model to calculate energy losses for at least 106 particles, and then plot the distribution as a histogram.

In this work, surface effects are taken into account when calculating the DIIMFP according to the dielectric theory of Drude [5]. When calculating the transmission function, it must be borne in mind that the ingress of an electron from a vacuum to a surface and the escape of an electron from a surface into a vacuum are two different processes that are described by two different formulas. In Fig. 1, *a* DIIMFP outside the layer of matter are shown, as can be seen when moving away from the surface of the layer, the DIIMFP of the process in which the electron falls to the surface decreases faster than the DIIMFP of the process in which the electron leaves the surface, this is explained by the presence of a surface charge. Fig. 2, *b* shows the dependence of the inverse IMFP, as can be seen from the graph, surface effects have a strong effect in the region of 10 Å on both sides of the boundary of the solid layer. It is important to note that the probability of an electron scattering and losing energy in a vacuum near the surface is not zero.

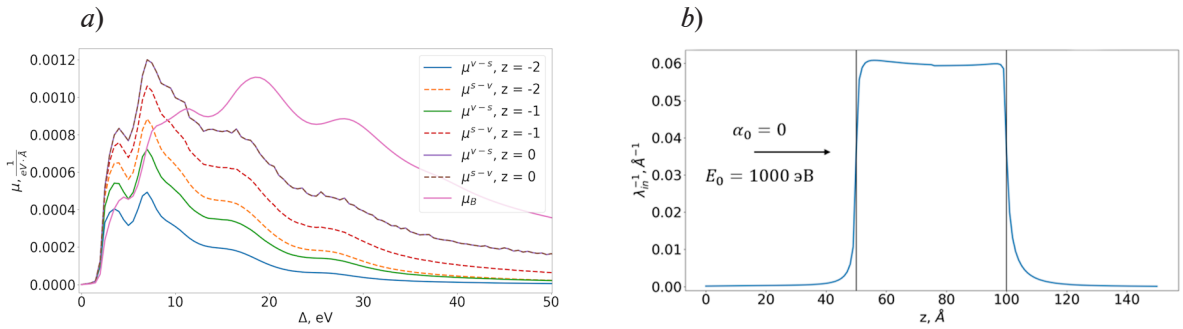

Fig. 1. Calculated DIIMFP for cases when an electron from a vacuum enters the surface of $\mu^{v\to s}$ and when an electron leaves the surface of $\mu^{s\to v}$. μ_B is the DIIMFP in the depth of the target ($z\to\infty$). The z coordinates are given in angstroms (*a*), the dependence of the inverse IMFP for an electron with an energy of 1000 eV in copper on the scattering coordinate. Vertical black lines show the boundaries of a solid (5 nm layer thickness) (*b*)

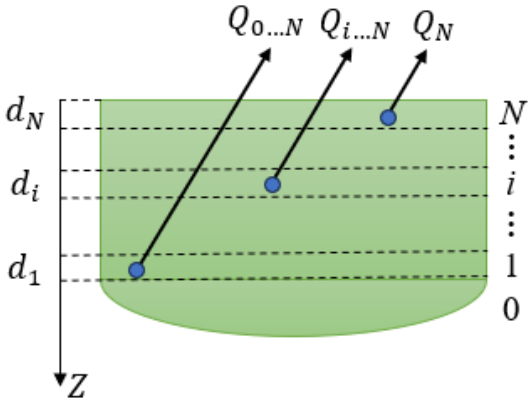

Fig. 2. Diagram of a multilayer target

When modeling the XPS spectrum, even from an unoxidized target, it is necessary to divide the layer into many homogeneous layers (Fig. 2.) in order to take into account, the surface effects. It should be noted that in this model there are layers that affect inelastic scattering, but in which no electrons are born, these are layers close to the surface of a solid body in a vacuum.

Results and discussion

Fig. 3, *a* show the transmission functions calculated by the matrix method and the Monte Carlo method. As can be seen from the graphs, the results obtained by these methods are in good agreement (the mean square deviation is $8.13\cdot10^{-4}$), which indicates the adequacy of the calculated and simulation models. For comparison, the transmission function is calculated using the universal Tougaard formula [6], which does not take into account surface effects, as can be seen from the graphs, these transmission functions are very different.

Fig. 3, *b* shows the simulated XPS spectra for the Cu 2p line with and without consideration of surface effects. Here, the matrix method and the Monte Carlo method also agree well, which indicates the adequacy of the calculated and simulation models (the mean square deviation for the spectrum, taking into account surface effects and without taking into account surface effects, are

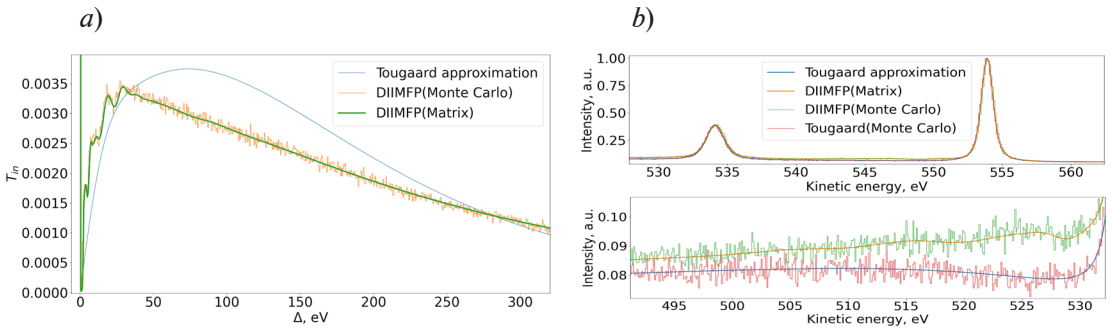

Fig. 3. Transmission functions calculated for a 5 nm thick copper layer. The electron energy is 1000 eV. Electrons fall to the surface normally (*a*), modeled XPS spectra of the Cu 2p line (*b*)

0.009 and 0.017, respectively). As can be seen from the graphs, the area of elastic peaks practically coincides, the qualitative difference is visible only for the background, because peaks appeared there due to the loss of energy by electrons to the excitation of surface plasmons.

Conclusion

The paper proposes a model of inelastic electron scattering based on the dielectric theory of Drude, taking into account surface effects. The matrix method and the Monte Carlo method showed good agreement, confirming the adequacy of the models. Consideration of surface effects significantly affects the energy spectra of XPS in the inelastic background region (the appearance of surface plasmons).

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