Simulation of e-beam penetration through multilayer structures

© S.S. Borisov¶, S.I. Zaitsev*

M.V. Lomonosov Moscow State University, Physical Department,
119992 Moscow, Russia
* Institute of Problems of Microelectronic Technology,
142432 Chernogolovka, Russia

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Using developed simulation in discrete loss approximation Monte-Carlo program we carried out analysis of secondary electrons energy spectra of multilayered structures. The possibility of determination of subsurface layers parameters using energy spectra of secondary electrons is shown as far as a way to avoid time consuming Monte-Carlo simulations for some cases.

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1. Introduction

Historically, the first approximation used in Monte-Carlo (MC) simulations was the continuous loss approximation (CLA). In this approximation energy looses are described by the average stopping power (usually using Bethe formula) — it is assumed that electron looses energy continuously along the trajectory. This approximation can be also called an average loss as it is assumed that losses along a small trajectory part are not random, but equal to the average value. The electron flight direction is usually assumed to change at the elastic interaction points.

The simulation models of CLA and discrete loss approximation (DLA), used for simulations in present work, are described in details in [1].

It can be shown (Fig. 1) that CLA does not allow an accurate description of scattering in solids. As an example CLA gives completely wrong secondary electrons (SE) shoot energy spectra (ES) for thin Au films (Fig. 1). That's why in the simulation program another approximation — discrete loss one — was used. Simulation algorithm takes into account all significant interactions (elastic, inner and outer atomic shell ionization plasmon excitations) separately in contradiction to CLA. In DLA electron losses energy by random parts in correspondence to the differential interaction crossections at the points of interaction. In fact DLA MC method becomes a truly imitational one.

Analysis of the CLA in which one neglects statistical properties of energy losses shows [2] that CLA is never valid in our case! It can be easily shown using Landau results on energy losses distribution deviation of electrons transmitted through a thin film of thickness x. One can see that ratio of mean-square losses σ_Δ to the mean energy losses ΔE (variation coefficient) [3]:

$$\frac{\sigma_\Delta}{\Delta E} = \sqrt{\frac{R}{xL_{\text{ion}}}}, \quad L_{\text{ion}} \approx \ln\left(1.16\,\frac{E_0}{J}\right),$$

is always greater than 1. Here R — electron range in solid, J — so-called effective ionization potential (some tenth-hundreds eV, so ionization logarithm L_{ion} value is about 5). As long as the distance between elastic interactions is rather small ($x \ll R$) Landau method can be used for analysis of MC algorithm. From the mentioned above one can see that statistical dispersion of energy losses is higher than the mean value and CLA is never valid.

Though the variation estimation raises no doubt, it is useful to compare (Fig. 1, Fig. 2) simulation results with the experimental losses spectrum of electron transmitted trough a thin film [4]. One can see that spectrum computed in CLA is in disagreement with the experimental one (Fig. 1). The contradiction is large enough so that the correct energy spectrum computation model upgrade is needed.

One can see that CLA gives results qualitatively wrong due to the forbidden energy region. In CLA electron cannot loose energy less then value of $E = \int_0^l \frac{dE}{dx}\,dx$, where l — film thickness, and energy spectrum is formed by the electron range distribution while in DLA energy loss fluctuation pays an important role.

Energy loss fluctuations resulted by inelastic loss during electron transmission through a thin film were described for the first time in [3]. They are ruled by the asymmetric uni-

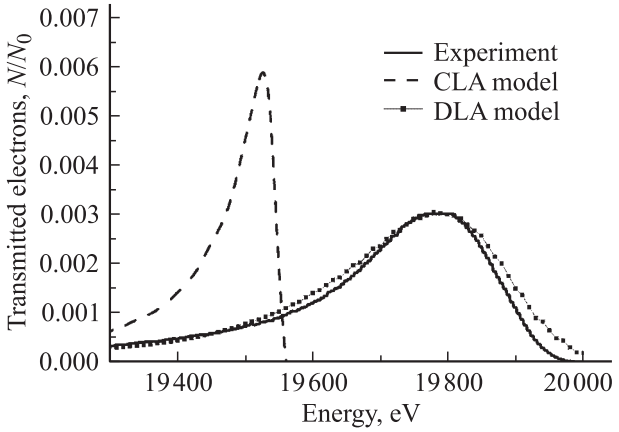

Figure 1. Comparison of the transmitted electron spectrum obtained using different approximations with the experimental data [4].

¶ E-mail: sergebor@mail.ru

versal Landau distribution (1) which can be characterized by narrow peak and long „tail“ in the positive parameter values region (due to a small interaction number each of which with a small probability transfers comparably large energy amount)

$$\Phi(\lambda) = \frac{1}{2i\pi} \int_{c-i\infty}^{c+i\infty} \exp\big(e\log(y) + \lambda y\big) dy. \qquad (1)$$

Here λ — dimensionless parameter proportional to the energy losses, c — some positive number.

As one can see from Fig. 3 shoot ES of SE computed by DLA (and experimental one, as they are very close) is well described by Landau distribution function.

For the Landau distribution function deduction, several admissions were made. For example, for small interaction numbers and thus low energy losses, so this distribution is valid for rather thin films in which energy losses are small in comparison to the electron energy. Furthermore fact of the presence of losses with discrete spectrum (plasmon excitations) was not taken into account. In the case of presence of such losses processes ES of electrons

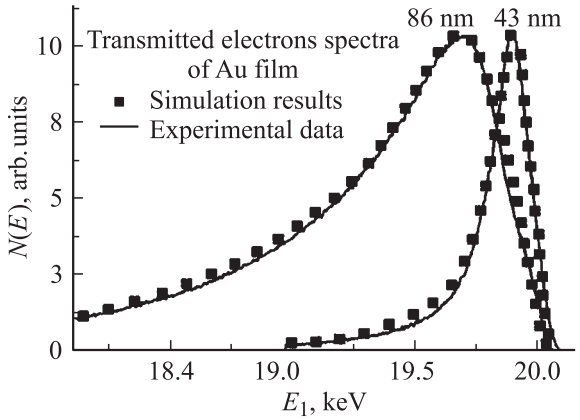

Figure 2. Comparison of the transmitted electron spectrum obtained by DLA with the experimental data [4].

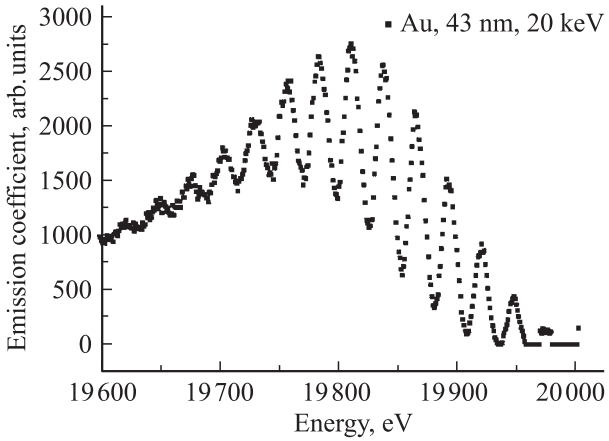

Figure 3. Transmitted electrons energy spectrum with the plasmon peaks.

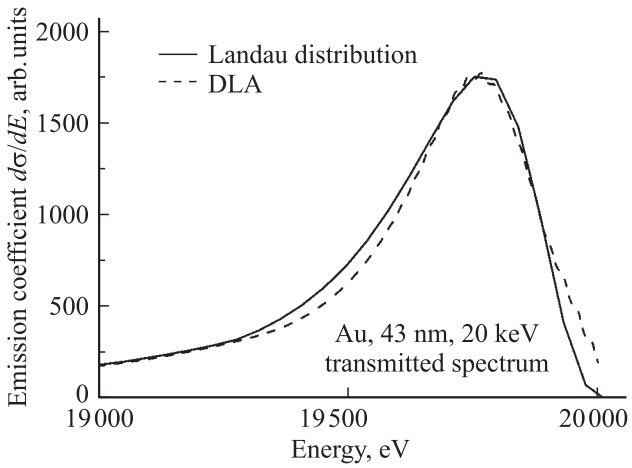

Figure 4. Comparison of DLA results with the Landau distribution function.

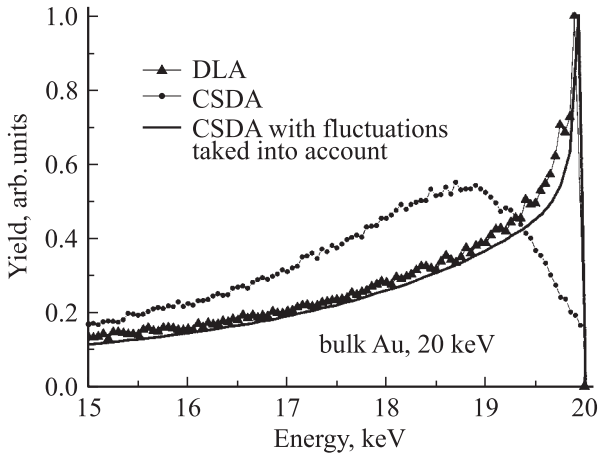

Figure 5. Bulk Au backscattered spectra obtained using DLA, CSDA and CSDA with fluctuation taked into account.

transmitted through a thin enough film has the structure shown on Fig. 3 — with peaks corresponding to 1, 2, 3.. plasmons. Such peaks are smoothed for thicker films due to the loss process with continuous spectrum. So Landau distribution function cannot simulate too thin film spectrum structure. For Au film one can see such spectrum structure up to thickness of 30–50 nm in simulation results. In the experimental data such structure can expire for thinner films due to the observation conditions.

Comparison of ES for Au films 30–200 mn thick (Fig. 4) shows that simulation using DLA results fits well to the Landau distribution function especially smoothed with a step higher than the plasmon energy.

CSDA can be modified to take into account energy loss fluctuations by specifying energy losses as a random quanttity and raffle it on each step. In this case results given by such code coincides well with the results of DLA. On Fig. 5 the backscattered from Au sample electrons spectrum is shown. One can see that modified CSDA and DLA gives

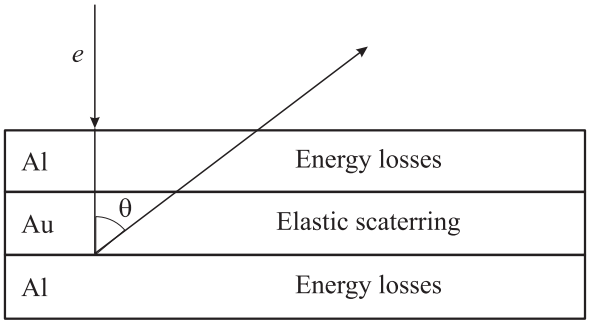

Figure 6. Scattering scheme in layered structure.

close spectra, while not modified CSDA cannot simulate such spectra detail as peak near beam energy [1].

Another interesting fact is that spectrum of multilayered structure like on Fig. 6 can be evaluated (without fine structure — plasmon peaks) as a composition of bulk substrate spectrum and Landau distribution function (Fig. 7), so one can use analytical models instead of time consuming Monte-Carlo for thin layers.

2. Monte-Carlo simulations of signal from multilayered structures results

With the advent of instruments dedicated to the analysis of ES of reflected electrons with high-resolution ($< 1\%$) [5], diagnostic possibilities of raster electron microscopy were extended. So, the well-grounded hope of using spectra for solving tomographical problems appears.

As it was shown, ES of transmitted electrons, obtained using DLA, agrees qualitatively and quantitatively with experimental data. This fact allows one to simulate the electron beam scattering in complex heterogeneous media, obtain simulated pictures of multi-layer microstructures and surface shape in back-scattered and true secondary electrons in electron microscopy.

Let's consider the results of multi-layer structures SE ES simulation, for example for the structure at Fig. 7. In comparison, in Au the elastic interactions between electrons and atomic nuclei prevail, but in Al the electron energy losses due to ionization prevail. So, the scattering conditions are different in each material — when electron reaches Au layer, it begins to elastically scatter greatly. As there is an average length of electron free path corresponding for each energy range of SE ES, each range carries information about the transmitted layers, the spectra are summed up in some way. At an example at Fig. 7 buried layer has essentially larger coefficient of reflection, and as one can see at ES in the range of energies corresponding to the depth of this layer peak emerges. The area of difference between spectra of structures without that buried layer and with it, obviously, is proportional to the layer thickness, and the position of additional peak maximum points to depth of the layer.

Therefore, subtracting the spectrum of Al from some structure spectrum, one obtains a curve which can used for estimating: the depth of layer by using the position of ES maximum and of the thickness of the layer — by the area under curve. As we can calculate these parameters of the ES *a priori* for specified topology, the possibility of measuring some parameters (as a thickness, a depth of lying or a type of material) of thin buried layers appears.

In Fig. 8 there is a group of spectra, corresponding to three-layer structures, consisting of 150 nm layer of Al, layer of Au with thickness of 5–65 nm, and Al substrate, obtained using DLA. At Fig. 9 there are analogous curves, obtained using CLA. The difference caused by forbidden losses zone is clear.

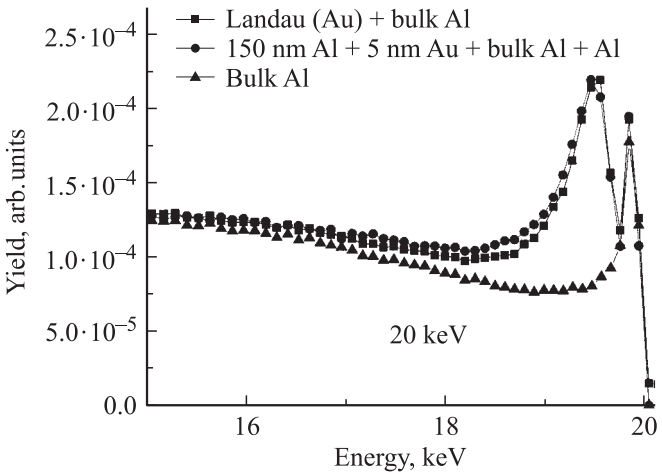

Figure 7. Spectra of structure decomposited into spectrum of bulk substrate and Landau distribution function.

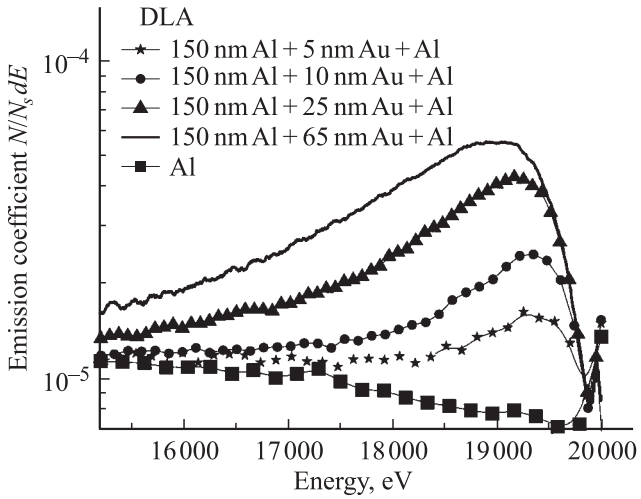

Figure 8. Backscattered electrons spectra of a three-layer structures, consisting of 150 nm layer of Al, layer of Au with thickness of 5–65 nm, and Al substrate. Discrete losses approximation results.

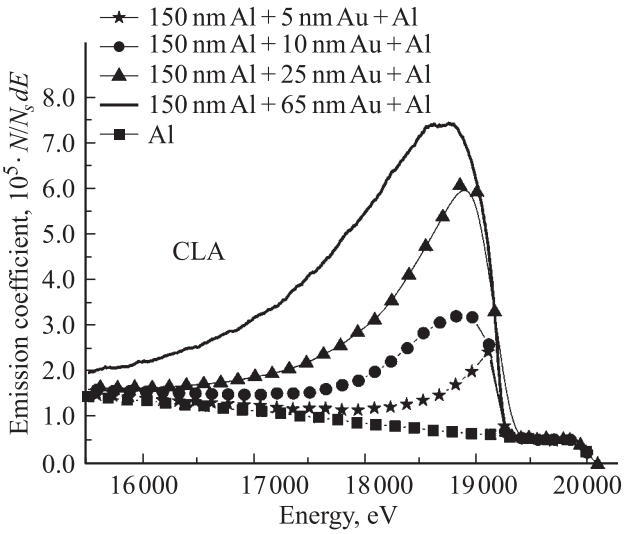

Figure 9. Backscattered electrons spectra of a three-layer structures, consisting of 150 nm layer of Al, layer of Au with thickness of 5–65 nm, and Al substrate. Continuous losses approximation results.

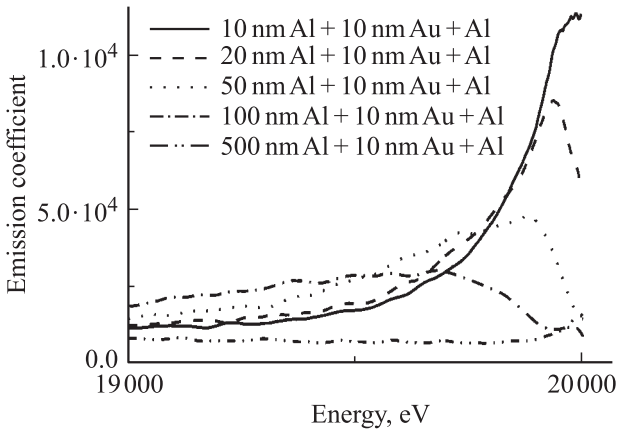

Figure 10. Backscattered electrons spectra for a case of variable thickness of covering Al layer (10–100 nm) and 10 nm Au layer on Al substrate.

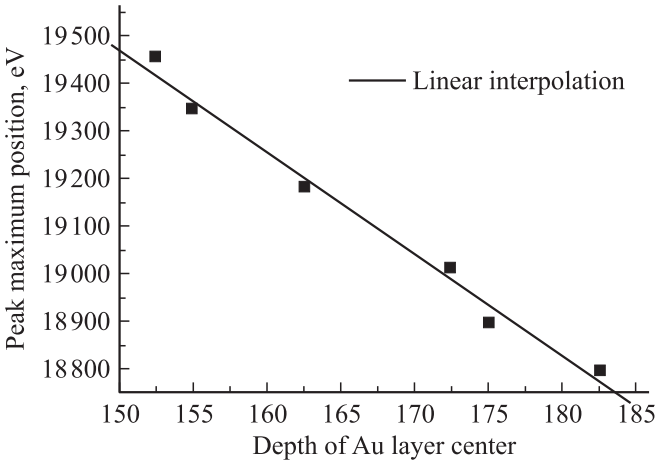

Figure 11. Dependence of backscattered electrons spectra maximum position of the covering layer thickness for a case of 10–100 nm Al layer on 10 nm Au lauer on Al substrate (Fig. 8).

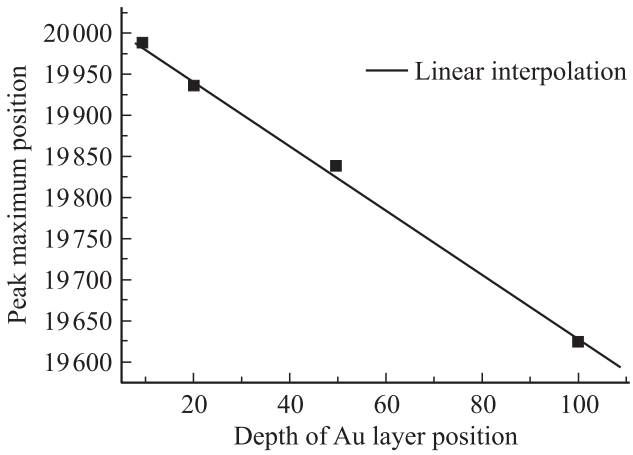

Figure 12. Dependence of backscattered electrons spectra maximum position of the Au layer thickness for a case of 150 nm Al layer on 5–65 nm Au layer on Al substrate (Fig. 6).

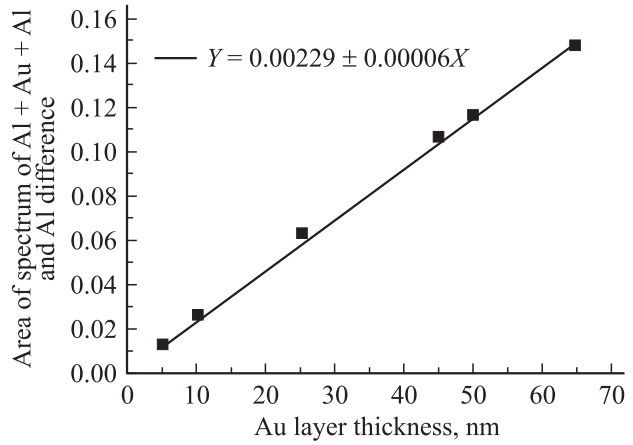

Figure 13. Dependence of backscattered electrons spectra peak corresponding to the Au layer of the Au layer thickness for a case of 150 nm Al layer on 5–65 nm Au layer on Al substrate (Fig. 6).

At Fig. 10 there is a group of spectra for a case of variable thickness of outer Al layer (10–100 nm) and layer of Au (10 nm) on Al substrate.

From Fig. 11 and 12 (where the positions of the Au layers centers for a case of variable thickness are shown) one can see that the dependence between positions of peak maximum is practically linear in wide enough range of thickness and is well described by the average loss. In Fig. 13 one can see that area of the spectrum difference is also in linear relation with the size of the buried layer.

3. Conclusion

For the quantitative measurement of layered structures parameters a simple model is presented. The model is valid if the depth of inner-layer is less than the transport length of fast electrons in light material and if the thickness of the layer is less than the transport length of fast electrons in

heavy material. The obtained dependencies allow measuring thickness and depth of subsurface structure, and in a case of presence of information about structure geometry — allow determined the type of composing material. On demonstrated example, it is possible to observe and measure parameters of layer with thickness down to 1 nm of Au layer under 150 nm layer of Al.

Another useful fact is that the energy spectrum of electrons transmitted through a thin film can be described by analytical formula with high accuracy, which gives an opportunity to predict energy spectrum for the multilayered structures not involving the time consuming clumsy Monte-Carlo algorithm. For the cases considered above, the energy spectrum can be described as sum of the substrate spectrum an transmission spectrum of the covering layers.

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