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Monte Carlo Method in Scanning Electron Microscopy. 3. Modern Condition of the Problem

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Abstract—The applicability of the Monte Carlo method for modeling images obtained in a scanning electron microscope is assessed. It is shown that in the Monte Carlo method, it is impossible to take into account all the mechanisms of the interaction of electrons with matter that affect image formation. Modern random-number generators create an insufficient amount of random numbers necessary for modeling the scattering of electrons in matter. The time it takes to modeling images using contemporary personal computers is too long: it takes years of continuous computer operation. There is no evidence of correctness of the results of the Monte Carlo method when generating images. These factors prove the impossibility of using the Monte Carlo method to modeling the scattering of electrons in a solid, which is used in image formation in a scanning electron microscope.

Keywords: Monte Carlo method, statistical modeling, random numbers, scanning electron microscope, SEM, virtual scanning electron microscope, modeling of electron trajectories, image formation

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INTRODUCTION

Scanning electron microscopy is widely used in various fields of science and technology [1–5]. It has been most common in microelectronics and nanoelectronics [3–5] for measuring the linear dimensions of chip elements [3–6], the critical (minimum) dimensions of which are currently 14 nm. Special scanning electron microscopes (SEMs) for measuring the critical dimensions of chip elements, called CD-SEM (Critical Dimension Scanning Electron Microscope) have been produced. At present, sizes of up to 30 nm can be measured using SEM [6, 7]. Attempts are being made to measure smaller dimensions using the Monte Carlo method [8–13] and a virtual scanning electron microscope (VSEM) [7, 14–18].

Virtual scanning electron microscopes [14–18] belong to virtual instruments [14]; they are made based on an imitator or a simulator [15]. It was shown that a VSEM could not be created based on an imitator (modeling of SEM operation using the Monte Carlo method) [15]. A virtual SEM was created [17] based on a simulator, simulating an image analogous to the image obtained by a real SEM using an analytical model [16] of SEM image formation.

In [19], the results of modeling of SEM signals by the Monte Carlo method and experimental signals did not coincide with each other in all parameters of the structures studied and signals of the scanning electron microscope. Unaccounted for contributions of secondary electrons, the consideration of a number of physical mechanisms for the production of secondary electrons, and the mechanisms of electron (primary and secondary) interactions with matter in the modeling were cited as the reason for this discrepancy [20]. Possible changes in the Monte Carlo method for eliminating these shortcomings and modeling SEM images similar to real ones were also considered. However, attempts to eliminate the shortcomings lead to a significant increase in the modeling time [20], bringing it to tens or more years of continuous operation of a personal computer, while not guaranteeing the final result, that is, the coincidence of the model and real images of relief structures.

Recently, the mechanisms of SEM image formation in the collection of backscattered electrons were studied [21–25]. The results of these studies can have a significant impact on development of the Monte Carlo method in the practice of scanning electron microscopy.

This paper is the continuation of a series of articles [19, 20]. Here, we discuss the effect of the results of [21–25] on modification of the Monte Carlo method for its application in scanning electron microscopy.

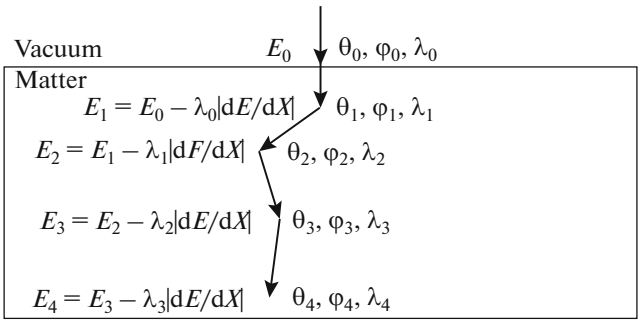

Fig. 1. Schematic diagram for Monte Carlo modeling of trajectory of an electron in matter.

THE MONTE CARLO METHOD IN SCANNING ELECTRON MICROSCOPY

The method of statistical modeling (the Monte Carlo method) is a general mathematical method. This makes it possible to apply it both in science and in other areas of human activity [26]. The method is also used in scanning electron microscopy [8–11, 27]).

However, the application of the Monte Carlo method to scanning electron microscopy in the manner that is implemented in [8–11, 27] is incorrect. It is demonstrated in [19] that the results of the modeling of SEM signals by the Monte Carlo method do not correspond to the results obtained using a scanning electron microscope, for all parameters of the signals and the microscope. Attempts to modify the Monte Carlo method [20] do not give any result because of insufficient knowledge of secondary-electron generation mechanisms and the mechanisms of electron (primary and secondary) interaction with matter, insufficient volume of random numbers, and an extremely long modeling time when using personal computers.

Attempts to solve some of these problems were carried out in [21–25]; namely, image-formation mechanisms in a scanning electron microscope operating in the mode of the collection of backscattered electrons were studied. The results give a new viewpoint on application of the Monte Carlo method in scanning electron microscopy.

Schematic diagram of the Monte Carlo method. Application of the Monte Carlo method in scanning electron microscopy is based on the modeling of electron trajectories in matter [1, 8, 9, 19, 28]. The schematic diagram of such motion, used in the Monte Carlo method [1, 19, 28], is presented in Fig. 1. The diagram is analyzed in detail in [19]. Two physical phenomena are used here: the elastic scattering of electrons at atomic nuclei and the energy loss of an electron for the ionization of atoms of which the substance consists. The bremsstrahlung emitted by an electron in the field of the atomic nucleus, which is the third fundamental process of the interaction of electrons with matter and the contribution of which is sufficiently large, is usually not taken into account.

Elastic scattering of electrons. The elastic scattering of electrons at atomic nuclei is described in the diagram (Fig. 1) by the mean free path λ, which is determined by the equation

$$\lambda = \left(N_A \rho \sum_i C_i \sigma_i / A_i \right)^{-1}, \quad (1)$$

where N_A is Avogadro's number, ρ is the density of matter, A_i is the atomic weight, C_i is the specific concentration of atoms, and σ_i is the total cross section for elastic scattering at atoms of the ith type.

For the total elastic scattering cross section, different equations are used. Usually [27, 28], the total scattering cross section is determined by an expression describing the scattering of electrons at a screened atomic nucleus, that is,

$$\sigma = \frac{\pi e^4 Z(Z+1)}{4E^2 \beta(\beta+1)}, \quad (2)$$

obtained by integrating the differential cross section of elastic scattering, determined by the Rutherford formula, taking into account the screening effect of the charge of the atomic nucleus. This formula has the form of [28]

$$\frac{d\sigma}{d\Omega} = \frac{Z(Z+1)e^4}{16E^2\left(\sin^2\theta/2 + \beta^2\right)^2}, \quad (3)$$

where e is the charge, E is the electron energy, θ is the scattering angle, β is the screening parameter of the charge of the atomic nucleus, and Z is the atomic number of the chemical element at the nucleus of which scattering occurs. In [27, 28], the following expression is used to calculate the screening parameter:

$$\beta = 5.43 Z^{2/3}/E, \quad (4)$$

where the electron energy E is taken in electronvolts.

The dependence of the electron mean free path in silicon on the energy is shown in Fig. 2.

Inelastic energy loss. The specific electron energy loss dE/dX in different activities is calculated using different equations. However, for high electron energies ($E > 1$ keV), the energy loss is usually determined by the Bethe equation [27, 28], which describes the average energy loss for the ionization of atoms in a matter of complex composition.

$$\frac{dE}{dX} = -\frac{2\pi e^4 \rho N_A}{E} \sum_i \frac{C_i Z_i}{A_i} \ln\left(1.166E/J_i\right), \quad (5)$$

where e is the electron charge, ρ is the density of the substance, E is the energy of the incident electron (eV), N_A is Avogadro's number, A_i is the atomic weight, Z_i is the atomic number, C_i is the specific con-

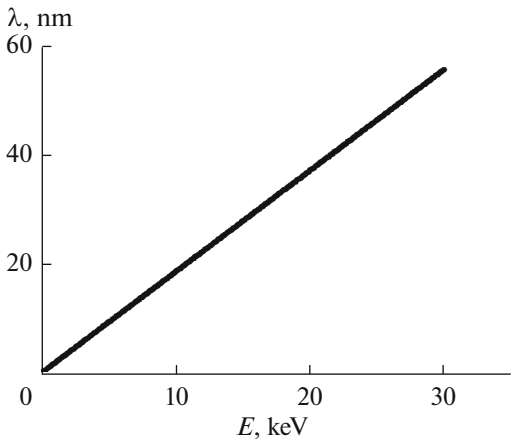

Fig. 2. Dependence of the mean free path of electrons on the energy in silicon.

centration, and J_i is the average ionization potential (eV) of the ith type, described by the expression

$$J_i = 11.5Z_i. \quad (6)$$

The average ionization potential determines the average energy needed to form a pair of electron–ion particles. For silicon, the average ionization potential is 161 eV.

The dependence of the average ionization loss of electrons in silicon on the energy is shown in Fig. 3.

Features of the diagram of the Monte Carlo method. Let us note some features of the schematic diagram of the Monte Carlo method, presented in Fig. 1. To do this, we calculate the energy loss over the mean free path, that is,

$$\Delta E = \lambda \left| dE/dX \right|. \quad (7)$$

Here λ is determined by Eq. (1) taking into account Eqs. (2)–(4), and dE/dX is defined by Eq. (5) with Eq. (6) taken into account.

Curve *1* in Fig. 4 shows the dependence of the electron energy loss ΔE in silicon on its energy. We plot the average ionization potential of silicon on this graph (line *2*). It is clearly seen that the energy loss over the mean free path is much smaller than the average ionization potential. This means that the energy loss to ionization does not occur with each electron scattering event.

Let us calculate the distribution of the electron energy loss over the mean free path by the Monte Carlo method. It was demonstrated [20] that the Monte Carlo calculation of the average values of the energy loss (the points in Fig. 4) is in good agreement with the analytical calculation (curve *1*), which indicates the correctness of the results obtained in this case by the Monte Carlo method.

Therefore, the Monte Carlo method was used to obtain the distributions of the electron energy loss over

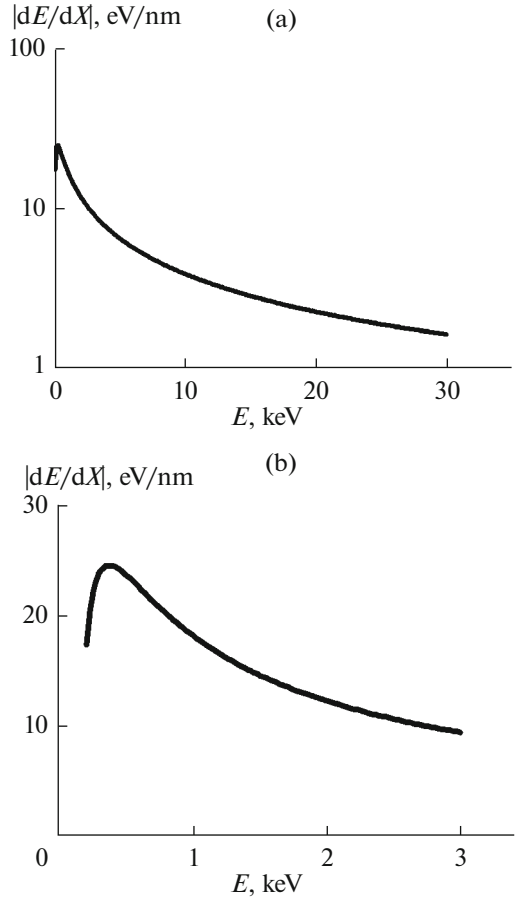

Fig. 3. Dependence of the ionization loss of electrons in silicon on their energy E in the regions of (a) high and (b) low energies.

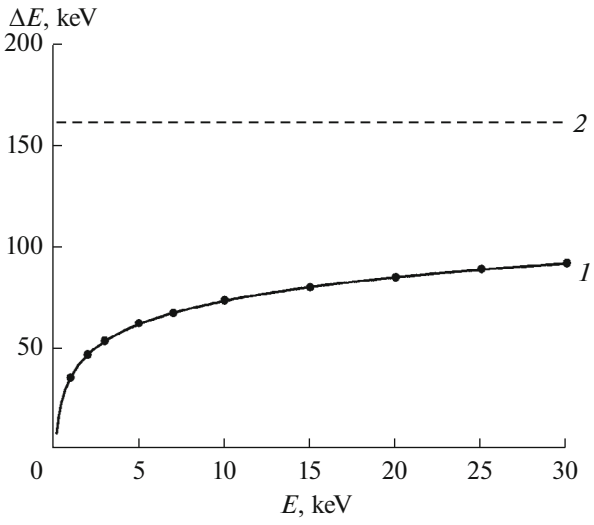

Fig. 4. (*1*) Energy loss over the mean free path of electrons in silicon for different electron energies; the points correspond to the average energy loss values modeling by the Monte Carlo method. (*2*) Average ionization potential in silicon.

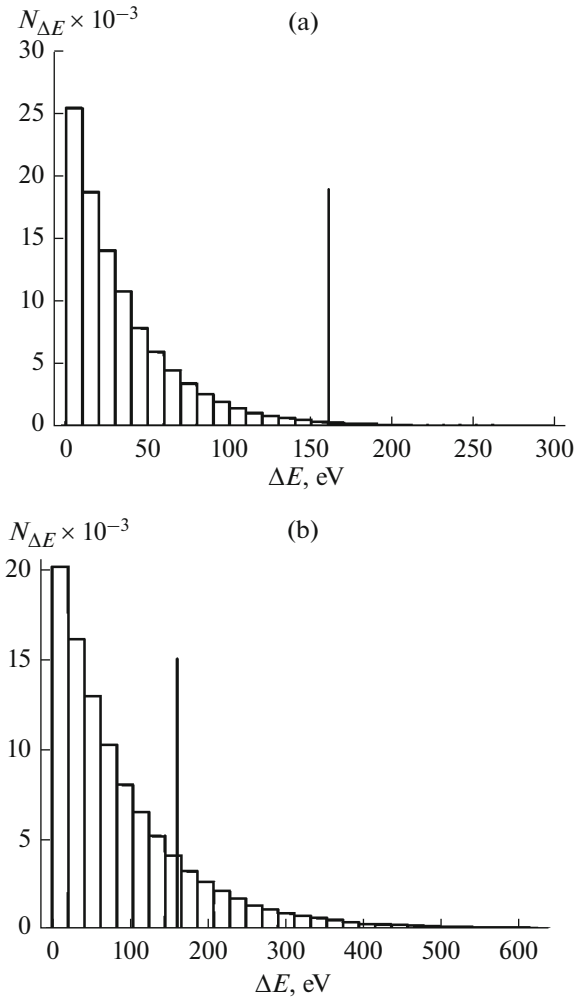

Fig. 5. Energy loss distributions over the electron mean free path in silicon, modeling by the Monte Carlo method, for electron energies of (a) 1 and (b) 30 keV. Vertical lines correspond to the average ionization potential of silicon.

the mean free path in silicon for electron energies lying in the range of 1–30 keV. The volume of statistics in each case was 100000. Figure 5 presents the histograms of these distributions for the electron energies of 1 keV (Fig. 5a) and 30 keV (Fig. 5b). Vertical lines in the histograms indicate the average ionization potentials of silicon. It is seen that only a small part of the collisions of electrons with atoms can ionize an atom. The dependence of the probability of exceeding the modeling energy loss over the mean free path above the ionization potential on the electron energy is presented in Fig. 6. Even in the best case (an electron energy of 30 keV), this probability is less than 20%. As for an electron energy of 1 keV, the probability is insignificant: it is less than 1%.

This means that the modeling diagram shown in Fig. 1 is not correct. It is not necessary to subtract the energy loss at every point of the trajectory fracture. Almost at all sites, only elastic scattering occurs, and

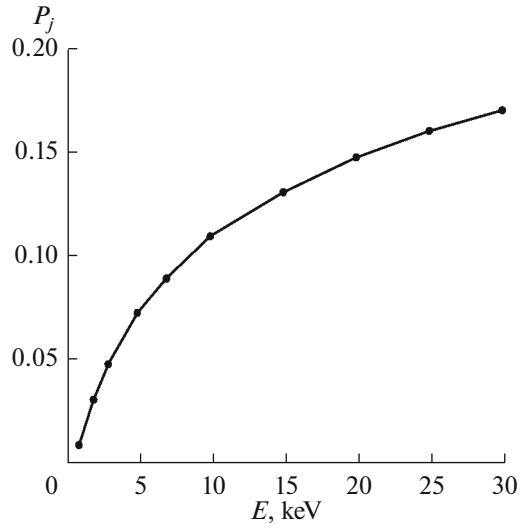

Fig. 6. Probability of exceeding the energy loss over the mean free path in silicon, modeling by the Monte Carlo method, of the ionization potential of silicon.

the mean free path is determined by elastic scattering (Eq. (1)). The energy loss must be taken into account only for one of the five scattering points at an electron energy of 30 keV and for one of the hundred points at an electron energy of 1 keV. The decrease in the electron energy must be taken into account only in the case when the energy loss exceeds the average ionization potential.

Thus, the modeling diagram shown in Fig. 1 does not correspond to reality and, therefore, cannot give in principle results that coincide with the experiment.

MECHANISMS OF SECONDARY-ELECTRON GENERATION

Taking into account the generation of secondary electrons in the Monte Carlo modeling of SEM images is applied very rarely because, as shown in [20], secondary-electron generation mechanisms are insufficiently studied, current generators are not capable of generating enough random numbers, and considering secondary electrons increases the modeling time sharply.

In the course of studies presented in [21–25], a new mechanism of secondary-electron generation was discovered. It consists of the scattering of primary electrons at conduction electrons [22, 25]. The contribution of this mechanism to the generation of secondary electrons is significantly (tens of times) greater than that of other mechanisms [22, 25]. Therefore, this mechanism must be taken into account, as well as the effect of secondary electrons themselves, on image formation.

The cross section for elastic electron scattering at an electron is not described by Eqs. (2)–(4), and the

mean free path, in this case, is not described by Eq. (1). Also, because of the proximity of the masses of a free electron and a conduction electron, elastic electron scattering at an electron leads to the appearance of two free electrons, each of which has a lower energy than the energy of the primary electron. The sum of the energies of both electrons is the same as the energy of the primary electron because the process is elastic Subsequent elastic scattering will again increase the number of free electrons by a factor of two. Therefore, the number of free electrons increases exponentially. The energy of these electrons decreases sharply (although the process of scattering is elastic) is also exponential on average.

This mechanism of primary electron scattering, which is observed for metals and electronic semiconductors, neither correspond to the modeling diagram (Fig. 1) nor can be described by Eqs. (1)–(6).

In the Monte Carlo method applied to metals and electronic semiconductors, it is necessary to modeling motion in the matter of both primary and (necessarily!) secondary electrons. The conduction electrons, having received energy, become free and participate in the process of forming a SEM image. In addition, it is necessary to take into account the density of conduction electrons and the bending of bands near the surface of semiconductors. Apparently, it is necessary to take into account the density of the electron distribution with respect to momentum, which depends on the doping of the substance and the presence of electrical contacts of metal films with semiconductor substrates [29].

MODIFICATION OF THE MONTE CARLO METHOD

To eliminate the shortcomings discussed in this paper and in [19, 20], it is necessary to separate the modeling of electron trajectories by the Monte Carlo method into two different methods. One method is used in modeling in dielectrics and *p*-type semiconductors, in which there are no conduction electrons; the other is applied in modeling in metals and *n*-type semiconductors, in which there are conduction electrons.

In the former case, the modeling diagram (Fig. 1) should be changed. It should be borne in mind that most of the collisions are elastic collisions. The energy loss should be subtracted only in the case that the modeling energy loss is higher than the average ionization potential.

In the latter case, the modeling is much more complicated. It is necessary to take into account the elastic scattering of a free electron (both primary and secondary) at conduction electrons. The problem of the scattering of a free electron at a free electron (the Möller process), which is close to the problem we need, is presented in textbooks on quantum electrodynamics [30]. However, the Möller equations are not suitable for the Monte Carlo modeling. To determine the mean free path, it is necessary to know the total scattering cross section. In this case, the Möller equations give an infinite value of the total cross section.

In the Rutherford formula (Eq. (2)), which is used in the former case, infinity is eliminated by introducing a shielding of the charge of the atomic nucleus (Eq. (4)) into the differential cross section (Eq. (3)). It appears that some infinity limiters of the total cross section should be introduced into the Möller equations. However, it is more advisable to solve the problem of electron scattering at conduction electrons.

It is necessary to take into account the modeling of the motion of secondary electrons in the latter case. This will lead to a sharp increase in the required number of random numbers and an increase in the modeling time [20]. It is also necessary to take into account the inelastic scattering of secondary (and primary) electrons at atomic nuclei, which leads to the appearance of secondary ionization electrons. It should be borne in mind that not every collision with an atom (as shown above) leads to the appearance of ionization electrons.

All these corrections lead to a sharp increase in the required volume of random numbers [20]. Therefore, new random number generators or, at least, methods for increasing the period of random numbers are needed. Modern personal computers do not have sufficient power [20] to perform modeling of the whole image using the Monte Carlo method. Therefore, a supercomputer is needed to solve such a problem.

Most importantly, in both cases, all the physical mechanisms that contribute to the formation of a SEM image should be taken into account in the modeling [19]. For this, it is necessary to compare the modeling with the experiment, at least as it was done in [19]. Only when the model and experiment yield comparable results will it be possible to consider the Monte Carlo method as a working tool in scanning electron microscopy. So far, it is too early for such a statement.

CONCLUSIONS

As follows from the preceding discussion and the results of [19, 20], all the works ([8–13] and others), using the modeling of SEM images by the Monte Carlo method, yield results that in principle cannot coincide with the experimental results.

All this creates the fundamental impossibility of using the Monte Carlo method in scanning electron microscopy for modeling images of micro and nanoobjects.

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