An Improved Monte Carlo Algorithm for Elastic Electron Backscattering from Surfaces*

Ivan T. Dimov, Emanouil I. Atanassov, and Mariya K. Durchova

Central Laboratory for Parallel Processing BAS, Sofia, Bulgaria
ivdimov@bas.bg, emanouil@copern.bas.bg, mabs@cantor.bas.bg

Abstract. The problen of the backscattering of electrons from metal targets is subject of extensive theoreticel and experimental work in surface analysis. We are interested in the angular distribution of the backscattered electrons. The flow of electrons satisfies an integral equation, which might be solved by Monte Carlo methods. The Monte Carlo approach, used by A. Dubus, A. Jablonski and S. Tougaard in their paper "Evaluation of theoretical models for elastic electron backscattering from surfaces" (1999), is based upon direct simulation of the physical process. We introduce different weights in the Monte Carlo algorithm, which decrease the variance. We also introduce artificial absorption probability and demonstrate significant improvements in the efficiency of the algorithm. Results of extensive numerical tests are presented.

1 Introduction

We consider the distribution of the "elastically backscattered" electrons, when a monoenergetic beam of electrons is bombarding a metal target. Studying the distribution of the emitted electrons with the same energy as the incident electrons is important for many experimental techniques, like *disappearance-potential spectroscopy, high-energy appearance potential spectroscopy, scanning electron microscopy* and others (see, e.g., [8,5,4]).

Usually the solid is considered as a homogeneous semi-infinite medium. The electrons undergo elastic collisions with the randomly distributed ionic cores, and the inelastic collisions are interpreted as absorption events, since only in the distribution of the same energy electrons is considered. Therefore the electron transport problem is a monoenergetic one. In [1] the problem is formulated in terms of a Boltzmann equation and then many different numerical methods are compared. The Monte Carlo approach is considered as one of the most accurate ones from theoretical viewpoint. However, in order to decrease the statistical error, long computational times are needed. Having the FORTRAN sources of the programs, used for the Monte Carlo computations in [1], we were able to substantially reduce the computational times, needed to obtain results with the same statistical error.

* Supported by Ministry of Education and Science of Bulgaria under Grant # MM 902/99 and by Center of Excellence BIS-21 grant ICA1-2000-70016

S. Margenov, J. Wasniewski, and P. Yalamov (Eds.): ICLSSC 2001, LNCS 2179, pp. 141–148, 2001.
© Springer-Verlag Berlin Heidelberg 2001

2 Overview of the Problem

We consider the electron transport problem, when a metal target is bombarded by a beam of electrons, and we are only interested in the flow of electrons with the same energy as initially. In [1], using the fact that the problem is monoenergetic, the target is homogeneous, etc., it is shown that the flow of electrons $\Phi(z, \overline{\Omega})$ satisfies the following simplified form of the Boltzmann equation:

$$\mu \frac{\partial \Phi\left(z, \overline{\Omega}\right)}{\partial z} + \Sigma_t \Phi\left(z, \overline{\Omega}\right) = \int\limits_{4\pi} \Sigma_s(\overline{\Omega}^{'} \rightarrow \overline{\Omega}) \Phi(z, \overline{\Omega}^{'}) d\overline{\Omega}^{'}, \tag{1}$$

where $\mu = \overline{\Omega}\,\bar{l}_z = cos\theta$ is the cosine of the angle of the electron direction with respect to the inward normal to the surface $\bar{l}_z$. The total cross-section Σ_t (inverse mean free path) and the scattering cross-section Σ_s are constants, specific to the material of the solid. The boundary condition describes the incoming flux of electrons:

$$\Phi\left(0, \overline{\Omega}\right) = \frac{J_0}{|\mu_0|} \delta(\overline{\Omega} - \overline{\Omega}_0), \qquad \overline{\Omega}\,\bar{l}_z \geq 0,$$

corresponding to the interaction on the boundary vacuum - solid ($\overline{\Omega}_0$ is the initial angle). Such an equation may be transformed into an integral equation of the form $\Phi = K\Phi + \Phi_0$, as one can see for instance in more general setting in ([2], p. 169–173). When Φ depends on 6 variables - $r = (x, y, z)$ for the position and $\omega = (\omega_1, \omega_2, \omega_3)$ for the direction of the electron, the integral equation has a kernel

$$K(r', \omega', r, \omega) = \frac{\Sigma_s g(\mu) \exp(-\Sigma_t |r' - r|)}{2\pi |r' - r|^2} \delta\left(\omega - \frac{r - r'}{|r' - r|}\right), \; \mu = \frac{(\omega', r - r')}{|r - r'|}.$$

Since the problem is isotropic, as it was pointed out also in [1], the equations becomes two-dimensional, the variables are z and the angle w between the z-axis and the direction of the electron. In order to estimate the distribution of the backscattered electrons, we compute the integrals:

$$\int\limits_0^{\pi} \Phi(0, w) \psi_j(w) dw, \tag{2}$$

where $\psi_j(w) = H(w - a_{j+1}) - H(w - a_j)$, $j = 1, 20$, H being the Heaviside function, and $a_j = cos\left(\frac{4.5\pi(j-1)}{180}\right)$, $j = 1, 21$. This is equivalent to computing the following functional of the solution:

$$\int\limits_0^{\infty} \int\limits_0^{\frac{\pi}{2}} \Phi(z, w) \delta(z) \psi_j(w) dw dz. \tag{3}$$

In the following we consider only the case when the initial angle w_0 is π. However, the algorithm and the computer program can deal with any value of w_0.

The statistical error of a Monte Carlo algorithm for finding linear functionals of the solution of such an integral equation is measured by the variation of the corresponding random variables, if the estimates are nonbiased. Since in our case we are using 20 random variables, then the sum of all 20 variations measures the statistical error of the method, as in ([2], p. 161).

Sobol in ([11], p. 97) introduced the notion of *computational complexity* $C(A)$ of a Monte Carlo algorithm A (when the estimate is nonbiased and the rate of convergence $O(N^{-\frac{1}{2}})$ as the product of the (in our case cumulative) variation and the CPU time for realization of one instance of the random variable (in our case - trajectory).

The idea is that if one of the algorithms has 2 times smaller computational complexity than the other, than on the average 2 times less time is needed for the same accuracy. In the sequel we are going to compare the computational complexity of our improved algorithms with the original Monte Carlo algorithm of Dubus, Jablonski and Tougaard. Since CPU times are involved, this measure depends on the computer architecture. While we present results only for SGI Origin 2000, the same calculations performed on Intel Pentium processor yield similar results. For the comparisons we use the empirical value of the variation, obtained during the calculations. We note that this value is obtained with sufficient accuracy (apparently within 5 %).

3 Description of the Improved Monte Carlo Algorithm

In the sequel the letter U denotes a uniformly distributed pseudo-random number, taken from the pseudo-random number generator. We had two different approaches for generating suitable random variables. The first one is preferable when only one of the functionals has to be calculated, the second one when all 20 functionals are to be calculated with one run of the program.

1. Read initial data:
   (a) parameters of the problem - element's atomic number Z, energy of the electrons E (in eV), initial angle of the electrons w_0;
   (b) parameters of the algorithm - algorithm version -A.1 or A.2, absorption probability - constant or variable, absorption parameter ε, number of points N_{tr}.
2. Calculate some physical constants:
   (a) the elastic scattering cross-section σ_{el} is taken from the database and the mean free path λ is calculated as $\dfrac{1}{N\sigma_{el}}$, where N is the atomic density of the target. By σ_c we denote $\dfrac{1}{\lambda}$;
   (b) the inelastic mean free path (IMFP) $\lambda_{in} = \dfrac{E}{E_p^2\left\{\beta\ln(\gamma E) - \frac{C}{E} + \frac{D}{E^2}\right\}}$, where E_p, β, γ, C, D are taken from the database physical constants (see [12]), corresponding to the element's atomic number Z, and E is the energy of the electrons;

(c) the full scattering cross-section $\sigma = \sigma_c + \dfrac{1}{\lambda_{in}}$;

(d) load from database the arrays x_i and y_i, describing the distribution of the scattering angle.

3. The interval $\left[0, \dfrac{\pi}{2}\right]$ is divided into 20 sectors (α_i, α_{i+1}), $i = 1 \ldots 20$.

4. For $j = 1$ to N_{tr}:

(a) Set initial data

i. number of collisions $i = 0$;

ii. weight $W_0 = \dfrac{\sigma_c}{\sigma}$;

iii. the cosine of the initial angle with z-axis: $u_0 = -\cos w_0$;

iv. the z coordinate of the first collision $z_0 = -\dfrac{1}{\sigma u_0} \log U$.

(b) Calculate cosine of the new angle with z axis after the collision:

$$u_{i+1} = u_i \cos(\theta) + \sqrt{1 - u_i^2} \cos(\pi U) \sqrt{1 - cos^2\theta}.$$

where θ is the scattering angle. The FORTRAN procedure used by Dubus, Jablonski and Tougaard is applied for generating θ.

(c) Calculate the contribution of the collision to the functionals:

i. If the version is A.1, go to 4.3.2, if it is A.2, go to 4.3.3.

ii. For $k = 1$ to 20 calculate the contribution of the point to the k^{th} functional:

– choose random direction inside the k^{th} sector by generating a uniformly distributed angle ξ in the interval $[0, \pi)$ - $\xi = \pi U_1$, and a uniformly distributed angle w in the interval $[\alpha_k, \alpha_{k+1})$ - $w = \alpha_k + (\alpha_{k+1} - \alpha_k) U_2$.

– Calculate the scattering angle r by

$$r = \arccos\left(u_i \cos w + \sqrt{1 - u_i^2} \cos\xi \sin w\right)$$

if $u_i \neq 1$, else set $r = \pi - w$;

– calculate the azimuthal angle $\varphi = \arccos \dfrac{\cos w - u_i \cos r}{\sqrt{1 - u_i^2} \sin r}$;

– calculate the Jacobian of the change of variables:

$$J(\xi, w) = \left\| \begin{array}{cc} \dfrac{\partial r}{\partial w} & \dfrac{\partial \varphi}{\partial w} \\ \dfrac{\partial r}{\partial \xi} & \dfrac{\partial \varphi}{\partial \xi} \end{array} \right\|$$

$$\frac{\partial r}{\partial w} = -\frac{1}{\sin r}\left(-u_i \sin w + \sqrt{1 - u_i^2} \cos\xi\right),$$

$$\frac{\partial r}{\partial \xi} = \frac{\sqrt{1 - u_i^2} \cos\xi \sin w}{\sin r},$$

$$\frac{\partial\varphi}{\partial w} = \frac{\sin w - u_i \sin r \frac{\partial r}{\partial \xi} + \cot r \frac{\partial r}{\partial w}(\cos w - u_i \cos r)}{\sqrt{1-u_i^2}\sin\varphi \sin r},$$

$$\frac{\partial\varphi}{\partial \xi} = -\frac{(u_i - \cot r\,(\cos w - u_i \cos r))}{\sqrt{1-u_i^2}\sin\varphi \sin r}\frac{\partial r}{\partial \xi},$$

when $u_i = \pi$ the Jacobian $J(\xi, w)$ is 1;

– the density $p(r)$ is calculated by

$$p(r) = \frac{1}{200}\left(\left(\sqrt{\frac{1-\cos r}{2}} - x_l\right)\frac{y_{l+1}-y_l}{x_{l+1}-x_l} + y_l\right) \times \frac{\sin r}{(x_{l+1}-x_l)(y_{l+1}+y_l)\sqrt{2(1-\cos r)}},$$

where l is determined such that $r \in [\arccos(1-2x_l^2), \arccos(1-2x_{l+1}^2)]$.

– the contribution of the point to the k^{th} functional is

$$|J(\xi, w)|\, p(r) \exp\left(\sigma \frac{z_i}{u_i}\right) W_i$$

and is added to the estimator S_k go to (4.4).

iii. If the new direction, determined by the cosine is upwards (i.e. $u_{i+1} > 0$) then determine for which k we have $u_i \in [\arccos \alpha_{k+1}, \arccos \alpha_k)$ and add $\exp\left(\sigma \frac{z_i}{u_i}\right) W_i$ to the estimator S_k.

(d) Increase the number of collisions - $i = i + 1$.

(e) Calculate the new z coordinate of the electron, using the new cosine: $z_i = z_{i-1} + \frac{1}{\sigma u_{i-1}} \log U$.

(f) If $z_i < 0$ then the electron has gone out of the surface, so go to 4.

(g) If $i = 1$ we do not allow the electron to be absorbed, so set the new weight W_i equal to W_{i-1} and go to (4.11).

(h) Calculate the threshold h depending on the absorption type, $h = 1 - \varepsilon$, if constant absorption type, $h = \exp(\varepsilon z_{i-1})$ if variable.

(i) Compare random number U with h, and if it is smaller, go to 4.

(j) Change the weight: $W_i = \frac{W_{i-1}}{h}$.

(k) Set $W_i = \frac{\sigma_c}{\sigma} W_i$ and go to (4.2).

4 Numerical Experiments and Conclusions

This section contains results from the calculations of the distribution of the elastically backscattered electrons are presented in the following tables. Experiments are carried out for energies of the electrons 100, 500, 1000 and 5000 eV, and for targets made of Aluminum, Copper, Silver and Gold. The CPU times are from computations on SGI Origin 2000, using double precision floating point arithmetics. Similar improvement ratios were observed on Intel processors.

Table 1. The best results for each energy and atomic number.

Z	Alg.	E(eV)	Eps	Prob.	N_{tr}	D	$C(.)$	$C(Orig)/C(A)$	
13	Orig.	100			10^7	3.51E-02	1017	3.57E-06	
	A.1	100	0.2	var.	10^5	4.03E-04	23	9.30E-08	38
	A.2	100	0.3	var.	10^6	1.34E-02	15	1.96E-07	18
	Orig.	500			10^7	1.22E-02	1421	1.73E-06	
	A.1	500	0.1	var.	10^5	1.04E-03	22	2.32E-07	7
	A.2	500	0.4	const.	10^6	5.49E-03	19	1.05E-07	16
	Orig.	1000			10^7	5.56E-03	1634	9.09E-07	
	A.1	1000	0.4	const.	10^5	8.42E-04	29	2.47E-07	4
	A.2	1000	0.4	const.	10^6	2.72E-03	19	5.28E-08	17
	Orig.	5000			10^7	7.28E-04	1938	1.41E-07	
	A.1	5000	0.2	var.	10^5	2.64E-04	16	4.33E-08	3
	A.2	5000	0.3	var.	10^6	6.58E-04	11	7.49E-09	18
29	Orig.	100			10^7	4.91E-02	1029	5.05E-06	
	A.1	100	0.1	var.	10^5	1.67E-03	33	5.59E-07	9
	A.2	100	0.4	const.	10^6	2.22E-02	18	4.08E-07	12
	Orig.	500			10^7	3.90E-02	1277	4.98E-06	
	A.1	500	0.3	const.	10^5	6.97E-03	34	2.38E-06	2
	A.2	500	0.3	const.	10^6	2.32E-02	23	5.27E-07	9
	Orig.	1000			10^7	2.59E-02	1460	3.78E-06	
	A.1	1000	0.3	const.	10^5	1.22E-02	35	4.33E-06	0.9
	A.2	1000	0.3	const.	10^6	1.84E-02	23	4.30E-07	9
	Orig.	5000			10^7	4.82E-03	1869	9.01E-07	
	A.1	5000	0.2	const.	10^5	9.11E-03	52	4.74E-06	0.2
	A.2	5000	0.2	const.	10^6	4.23E-03	33	1.40E-07	6
47	Orig.	100			10^7	2.85E-02	1285	3.66E-06	
	A.1	100	0.1	var.	10^5	1.81E-03	38	6.89E-07	5
	A.2	100	0.1	var.	10^6	1.45E-02	26	3.77E-07	10
	Orig.	500			10^7	3.47E-02	1244	4.32E-06	
	A.1	500	0.4	const.	10^5	5.61E-03	28	1.55E-06	3
	A.2	500	0.4	const.	10^6	1.95E-02	19	3.65E-07	12
	Orig.	1000			10^7	2.82E-02	1373	3.87E-06	
	A.1	1000	0.3	const.	10^5	7.51E-03	35	2.60E-06	2
	A.2	1000	0.4	const.	10^6	1.97E-02	19	3.74E-07	10
	Orig.	5000			10^7	8.20E-03	1790	1.47E-06	
	A.1	5000	0.4	var.	10^5	9.16E-03	16	1.51E-06	1
	A.2	5000	0.3	const.	10^6	8.77E-03	24	2.10E-07	7
79	Orig.	100			10^7	1.97E-02	1406	2.77E-06	
	A.1	100	0.1	var.	10^5	2.18E-03	41	8.84E-07	3
	A.2	100	0.1	var.	10^6	1.11E-02	27	3.04E-07	9
	Orig.	500			10^7	2.67E-02	1331	3.55E-06	
	A.1	500	0.1	var.	10^5	6.40E-03	29	1.83E-06	2
	A.2	500	0.3	const.	10^6	1.53E-02	23	3.55E-07	10
	Orig.	1000			10^7	3.49E-02	1331	4.64E-06	
	A.1	1000	0.1	var.	10^5	1.82E-02	24	4.42E-06	1
	A.2	1000	0.3	const.	10^6	2.21E-02	23	5.07E-07	9
	Orig.	5000			10^7	1.72E-02	1688	2.90E-06	
	A.1	5000	0.2	var.	10^5	8.58E-02	17	1.50E-05	0.2
	A.2	5000	0.2	const.	10^6	1.55E-02	32	5.03E-07	6

Table 2. Numerical experiments for Copper, electron energy 100eV.

Alg.	Eps	Prob.	N_{tr}	D	Time	$C(.)$	$C(Orig)/C(A)$
Orig.			10^7	4.91E-02	1029	**5.05E-06**	
A.1	0.1	var.	10^5	1.67E-03	33	5.59E-07	9
A.1	0.1	const.	10^5	1.58E-03	67	1.06E-06	5
A.1	0.2	var.	10^5	2.34E-03	26	6.04E-07	8
A.1	0.2	const.	10^5	1.68E-03	42	7.04E-07	7
A.1	0.3	var.	10^5	9.52E-03	23	2.15E-06	2
A.1	0.3	const.	10^5	1.88E-03	32	6.01E-07	8
A.1	0.4	var.	10^5	7.71E-03	21	1.61E-06	3
A.1	0.4	const.	10^5	2.22E-03	27	5.89E-07	9
A.2	0.1	var.	10^6	1.88E-02	23	4.40E-07	11
A.2	0.1	const.	10^6	1.84E-02	44	8.17E-07	6
A.2	0.2	var.	10^6	2.30E-02	18	4.20E-07	12
A.2	0.2	const.	10^6	1.90E-02	28	5.38E-07	9
A.2	0.3	var.	10^6	3.06E-02	16	4.94E-07	10
A.2	0.3	const.	10^6	2.01E-02	22	4.40E-07	11
A.2	0.4	var.	10^6	4.34E-02	15	6.50E-07	8
A.2	0.4	const.	10^6	2.22E-02	18	4.08E-07	12

In Table 2 results for different values of the parameter ε of the two versions A.1 and A.2 and of the original algorithm are shown. In Table 1 the best computational results of both versions of our algorithm A.1 and A.2 are presented. In the tables one can see for each test the algorithm that was used, the elements atomic number, the absorption probability type - variable or constant, the number of trajectories used in the calculations, the empirical cumulative variance, the CPU time needed, the computational complexity of the algorithm and its ratio with the computational complexity of the algorithm of Dubus, Jablonski and Tougaard.

Figure 1 shows the results for the distribution of the backscattered electrons, when target is Gold, energy is 1000eV, and the number of trajectories is chosen so that the CPU time of the original and the improved Monte Carlo algorithm is made equal. The results of the experiments show that the proposed approach - adding an artificial absorption probability, controlled by the parameter ε,may lead to substantial improvement of the efficiency of the Monte Carlo algorithm. Although the first algorithm is in general less efficient than the second one, it has the advantage that when the value of only one of the functionals is needed, it requires about 5 times less operations, than for all 20, while the original one and the second algorithm requires almost the same number of operations, as for all 20. Taking this into account, it appears that if we are interested only in the flow of backscattered electron in certain direction, we should use version A.1, but if we need the distribution of electrons in all sectors, we should use version A.2. One can also see that the first version is more efficient when the energy of the electrons is smaller.

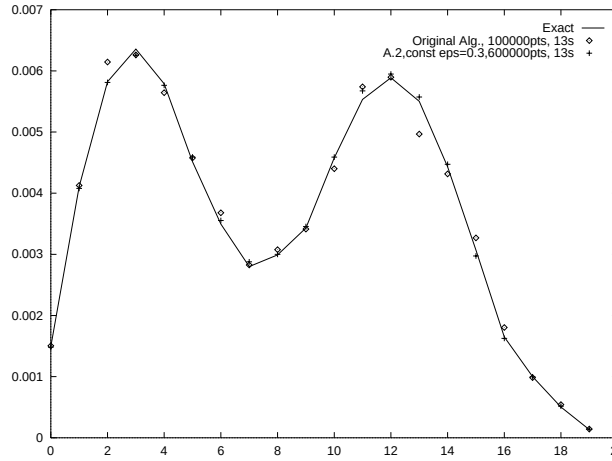

Fig. 1. Comparison of the results of the original and the new algorithm for Gold, electron energy 1000eV

Another observation is that in general when the atomic number is higher, lower values of ε should be used.

We also note that theoretically the estimate used by Dubus, Jablonski and Tougaard has small bias, since they assume that if an electron trajectory is more than 40λ, the eventual contribution of such electron to the functionals is neglectable. Our algorithm provides unbiased estimates.

References

1. A. Dubus, A. Jablonski, and S. Tougaard. *Evaluation of theoretical models for elastic electron backscattering from surfaces, Progress in Surface Science*, 1–41, 1999.
2. S. M. Ermakov and G. A. Mikhailov. *Statistical Modeling*, Moscow, Science, 1982.
3. G. Gergely. *Surf. Interf. Anal.*, 3, 201, 1981.
4. A. Jablonski. *Elastic Scattering and Quantification in AES and XPS*, 1989.
5. J. Kirshner and P. Staib. *Appl. Phys.*, 6, 99, 1975.
6. S. H. Overbury and G. A. Somorjai. *J. Chem. Phys.* , 66, 3181, 1977.
7. J. Pawluch and L. Eckertove. *Surf. Sci.*, 162, 896, 1985.
8. J. B. Pendry. *Low Energy Electron Diffraction: the Theory and its Application to Determination of Surface Structure*, Academic Press, London and New York, 1974.
9. C. J. Powell and A. Jablonski. *J. Phys. Chem. Ref. Data*, 28, 19, 1999.
10. R. Schmid, K. H. Gaukler, and H. Seiler. *Scanning Electron Microscopy*, 501, 1983.
11. I. M. Sobol'. *Numerical Methods Monte Carlo*, Moscow, Science, 1973.
12. S. Tanuma, C. J. Powell, and D. R. Penn. *Surf. Interf. Anal.*, 21, 165, 1994.