A New Weighted Monte Carlo Algorithm for Elastic Electron Backscattering from Surfaces ⋆

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Abstract

When a monoenergetic electron beam is bombarding a solid target, some electrons are elastically backscattered. This elastic electron backscattering effect plays an important role in many experimental techniques, like low-energy electron diffraction, scanning electron microscopy and others. Recently, the elastic peak has been used for the experimental determination of electron Inelastic Mean Free Paths (IMFPs) in the solid. This experimental determination (which is now considered as the most reliable [1]) consists in comparing the measurement to a model calculation in which the IMFP is a parameter. In most cases for the model calculation a simple nonanalog Monte Carlo simulation (where the inelastic events are considered as absorptions and taken into account by a weight) is used. In many cases, long computational times are needed, especially when the solid angle of the electron detector is small. In this work we introduce a different weighted Monte Carlo algorithm, which combines several techniques for variance reduction. Results of extensive numerical tests are presented, demonstrating the increased effectiveness of the new algorithm.

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1 Integral equation

The flow of electrons satisfies the integral equation

$$\varphi(x) = \int_X k(x', x)\varphi(x')dx',$$

where

$$k(x', x) = \frac{\sigma_{el} g(\mu, r') \exp(-\sigma|r' - r|)}{2\pi |r - r'|^2} \delta\left(\omega - \frac{r - r'}{|r - r'|}\right),$$

$$\mu = \frac{(\omega', r - r')}{|r - r'|},$$

$$\sigma = \sigma_{el} + \sigma_{in}.$$

In order to calculate a callibration curve, we need to solve the equation for several values of the IMFP $\lambda = \lambda_1, \ldots, \lambda_n$, setting $\sigma_{in} = \frac{1}{\lambda}$.

The term f corresponds to the intensity of the initial beam, which we consider coming from a point source. The equation is solved in the hyperplane $z > 0$. The detector is considered filling the space between two cones, outer cone with aperture angle α and inner cone with aperture angle β. One of the most popular types of detectors has inner angle zero and small outer angle - in the case of the spectrometer in Brussels it is around 12^o. We evaluate functionals of the solution, approximating the percentage of backscattered electrons. The percentage of backscattered electrons, registered by the detector after exactly n collisions, is equal to $\langle K^n f, h\rangle$, where the functional h represents the geometry of the detector. From other point of view this functional can be considered as a multi-dimensional integral. We need to calculate the sum of all these integrals for $n = 1, 2, \ldots$. We observe that if all the directions are fixed, and the paths obey the exponential distribution as required by the equation, integrals of this type can be solved in closed form, since only exponential functions are involved. However, our numerical experiments showed that for some combinations of directions the accuracy of the calculations is not enough, even when software for using extended precision is used, and such combinations are not rare. Therefore we decided to use the analytical formula for the integral only in the clear case, when all the directions are downwards, except for the last one. The yield coming from such electrons accounts for large percentage of the total yield, theoretically the variance decreases, since we reduce the dimensionality, and the computational time also decreases, since in this case the formula involves only multiplication, division and addition. We combine this approach with the introduction of an artificial absorption probability ε, as in ?? so that an electron has ε probability of being "absorbed" when there is a collision.

2 Algorithm Description

(1) Read initial data:
  (a) parameters of the problem: element's atomic number Z, energy of the electrons E, incidence angle u_0, detector position, aperture of the detector, inner angle of the detector, sequence of IMFPs - $\lambda_1, \ldots, \lambda_n$;
  (b) parameters of the algorithm: absorption parameter ε, number of trajectories N_{tr}.
(2) Preprocessing:
  (a) calculate the elastic scattering cross-section σ_{el} and the total cross-section σ using the database
  (b) load from database the arrays x_i and y_i, describing the elastic cross-section for this element and energy.
(3) For $j = 1$ to N_{tr}:
  (a) Set initial data
    (i) number of collisions $i = 0$;
    (ii) weight $W = \dfrac{\sigma_{el}}{\sigma}$;
    (iii) initial coordinates $w_0 = -\cos u_0$, $x_0 = \sin u_0$, $y_0 = 0$, $z_0 = 0$, $L = 0$;
    (iv) calculate the contribution of the point to the estimators:
      (A) select random angle $\overline{\Omega}$ within the detector ;
      (B) calculate the probability density $p(\Omega_0, \overline{\Omega})$ of changing the direction from $\Omega_0 = (x_0, y_0, w_0)$ to $\overline{\Omega} = (\overline{x}, \overline{y}, \overline{w})$, using the Jacobian

$$J(\xi, \chi) = \begin{Vmatrix} \dfrac{\partial \theta}{\partial \chi} & \dfrac{\partial \varphi}{\partial \chi} \\ \\ \dfrac{\partial \theta}{\partial \xi} & \dfrac{\partial \varphi}{\partial \xi} \end{Vmatrix}$$

$$\frac{\partial \theta}{\partial \chi} = -\frac{1}{\sin \theta} \left(-w_0 \sin \chi + \sqrt{1 - w_0^2} \cos \xi \right),$$

$$\frac{\partial \theta}{\partial \xi} = \frac{\sqrt{1 - w_0^2} \cos \xi \sin \chi}{\sin \theta},$$

$$\frac{\partial \varphi}{\partial \chi} = \frac{\sin \chi - w_0 \sin \theta \frac{\partial \theta}{\partial \xi} + \cot \theta \frac{\partial \theta}{\partial \chi} (\cos \chi - w_0 \cos \theta)}{\sqrt{1 - w_0^2} \sin \varphi \sin \theta},$$

$$\frac{\partial\varphi}{\partial\xi} = -\frac{(w_0 - \cot\theta\,(\cos\chi - w_0\cos\theta))}{\sqrt{1-w_0^2}\sin\varphi\sin\theta}\frac{\partial\theta}{\partial\xi},$$

(C) for each $\lambda_1, \ldots, \lambda_n$ calculate the probability $Q_i(\lambda_i, \Omega_0, \overline{\Omega}, z_0)$ of a particle with initial position (Ω_0, z_0) and position after the collision $(\overline{\Omega}, z_1)$ to have $z_1 < 0$:

- if for this electron the direction Ω has been always into the surface, use the formula:

$$Q = \prod_{j=1}^{i} \frac{\overline{w}}{(}\overline{w} - w_j$$

- otherwise, use the formula

$$Q = \frac{\exp\left(\frac{z_0\sigma}{w_1}\right)}{1 - \frac{w_0}{w_1}}$$

or

$$Q = \frac{\exp\left(\frac{z_0\sigma}{w_1}\right) - \exp\left(\frac{z_0\sigma}{w_0}\right)}{1 - \frac{w_0}{w_1}}$$

depending on wheter now Ω_0 points inside or outside of the surface, respectively.

- add $WQ\exp(-L(\frac{1}{\lambda_i} - \sigma_{el}))$ to the respective estimator, where $W_i = W\exp\left(-(\left(\lambda_i + \sigma_{el}^{-1}\right) - \sigma^{-1})L\right)$.

(v) calculate the new position (Ω', z') and update L:

- The new direction $\Omega' = (x', y', w')$ is obtained from the old one by:

$$x' = x\cos\theta + \frac{\sin\theta}{\sqrt{(y^2 + w^2)}}\left(-y^2 - w^2\right)\sin\varphi$$

$$y' = y\cos\theta + \frac{\sin\theta}{\sqrt{(y^2 + w^2)}}(w\cos\varphi + xy\sin\varphi)$$

$$w' = w\cos\theta + \frac{\sin\theta}{\sqrt{(y^2 + w^2)}}(-y\cos\varphi + xw\sin\varphi)$$

where θ and φ are the random scattering angle and azymutal angle (the azymutal angle is uniformly distributed in $(0, 2\pi)$ and the scattering angle has the appropriate distribution in $(0, \pi)$).

- The new z' is computed by

$$z' = z + \sigma^{-1} w \log u$$

Table 1
Results for Element Aluminum

Energy	Old	New	ε	Ratio
100	0.0013	1.70e-06	0.30	750
100	0.0018	2.80e-06	0.30	663
300	0.0011	3.00e-06	0.35	357
300	0.0017	3.90e-06	0.40	432
500	0.0008	2.20e-06	0.40	367
500	0.0012	2.80e-06	0.40	416
1000	0.0004	1.90e-06	0.40	223
1000	0.0006	2.90e-06	0.35	198

where u is uniformly distributed in $(0, 1)$.

(vi) if $z' < 0$, this point is out - go to 3;
(vii) if $i = 0$, set $i = i + 1$ and go to 3.1.4;
(viii) with probability ε this point dies and we go to 3, otherwise we set

$$W = \frac{\sigma_{el}}{\sigma} \frac{W}{1 - \varepsilon}$$

and go to 3.1.4.

3 Numerical Results

We compared our algorithm with the previously used algorithm. Both algorithms converge to the same estimates for the functionals, but with different statistical error. Since the experimenters observe yields, corresponding to values of σ_{in} close to the ones found in the database of Tanuma et al., we measure the efficiency of the algorithms by summing the empirical variance for the 5 closest to the database values of σ, and multiply it by the CPU time. As you will be able to see on the figure **??**, the calibration curve is approximately linear. Therefore this quantity is an accurate measure of the computational effort required for achieving given accuracy in determining the IMFP.

The figure **??** shows the results of the old and the new algorithm for a Copper target, energy 2000, aperture angle of 12 degrees and inner angle of zero. The initial beam goes in at 60 degrees and the detector is placed on the other side at 60 degrees. This data corresponds to an experimental situation, which might occur at the spectroscope at ULB, Belgium. Looking at the results on table 1, we see that the improvement ratio is 40 in this case. The value of the inelastic

Table 2
Results for Element Copper

Energy	Old	New	ε	Ratio
100	0.0038	1.03e-05	0.25	368
100	0.0055	1.40e-05	0.25	394
300	0.0013	1.23e-05	0.20	103
300	0.0018	1.58e-05	0.15	113
500	0.0012	2.07e-05	0.25	56
500	0.0019	2.84e-05	0.20	69
1000	0.0013	2.07e-05	0.25	64
1000	0.0021	2.84e-05	0.20	73
5000	0.0004	2.07e-05	0.25	20
5000	0.0006	2.84e-05	0.20	22

Table 3
Results for Element Silver

Energy	Old	New	ε	Ratio
100	0.0021	2.07e-05	0.25	104
100	0.0037	2.84e-05	0.20	129
300	0.0027	2.07e-05	0.25	131
300	0.0043	2.84e-05	0.20	151
500	0.0014	2.07e-05	0.25	67
500	0.0022	2.84e-05	0.20	77
1000	0.0007	2.07e-05	0.25	35
1000	0.0010	2.84e-05	0.20	36
5000	0.0006	2.07e-05	0.25	28
5000	0.0008	2.84e-05	0.20	27

mean free path, taken from the database of Tanuma et al., is therefore in the experiment an yield of around should be observed. On the figure, one can see how for the same computational time the new algorithm achieves around 6 times smaller error, which means that the old algorithm needs 36 times more computational time in order to achieve the same statistical error.

Table 4
Results for Element Gold

Energy	Old	New	ε	Ratio
100	0.0021	2.07e-05	0.25	103
100	0.0036	2.84e-05	0.20	129
300	0.0014	2.07e-05	0.25	66
300	0.0023	2.84e-05	0.20	81
500	0.0021	2.07e-05	0.25	101
500	0.0030	2.84e-05	0.20	105
1000	0.0022	2.07e-05	0.25	107
1000	0.0033	2.84e-05	0.20	116
5000	0.0007	2.07e-05	0.25	33
5000	0.0010	2.84e-05	0.20	34

4 Concluding Remarks

The results show that a significant improvement is possible when several techniques for variance reduction are applied. When the aperture angle of the detector is relatively small, the proposed approach makes possible on-line instead of batch processing.

The numerical tests suggest that the best values of ε are approximately inversely proportional to the mean number of collisions of the real electrons in the respective target. We note that the efficiency of the calculations is not very sensitive to the choice of ε.

The new algorithm performs better for energies of the electrons in the range $100 - 1000$, than for energies larger than 5000, probably due to the different shape of the elastic cross section.

References

[1] C.J. Powell and A. Jablonski, J. Phys. Chem. Ref. Data 28 (1999) 19.

[2] I.T. Dimov, E.I. Atanassov and M.K. Durchova, *An Improved Monte Carlo Algorithm for Elastic Electron Backscattering from Surfaces*