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Monte Carlo Technique of Simulation of Electron Motion in Gas

Andrey Trubitsyn and Victor Gurov

Department of Electronics, Ryazan State Radio Engineering University, Ryazan, Russia.

The present paper describes a numerical model of electron motions in the gas media. The respective software module is integrated into the copyright software designed for a numerical research of electron optic systems [1]. Experimental testing of the developed model is performed.

There are the following tasks: design of ion sources with electron impact, study of the effect of residual gases on electron microscopes and spectrometers etc. Their solution consists in determination of spatial configurations and kinematic characteristics of electron beams spreading in the gas media.

Mobility of electrons in plasma is higher in hundreds and even thousands times than mobility of ions. Therefore influence of external electromagnetic fields on physical processes occurring in plasma is determined and described by the motion of electrons. Specificity of the electron motion is generally set by processes of their collisions with gas molecules.

Numerical methods of the macroparameter determination for a certain process according to known microparameters are based on the Monte-Carlo technique. This method consists in sampling of these microparameters and carrying out a great number of statistical tests.

The length of an electron free path as an average distance passing by an electron between two successive collisions with gas molecules under the first approximation can be evaluated according to the following formula:

$$\lambda_0 = \frac{4kT}{\pi P d^2} \tag{1}$$

where P is the gas pressure, k is the Boltzmann's constant, T is the gas temperature and d is the molecule diameter [2].

More accurate models of collisions require taking into account dependence of a free path length on energy E, $\lambda_E = \lambda(E)$. According to the physical sense there is an inverse proportionality of an electron free path length to a total cross-section of scattering on gas molecules, i.e. $\lambda(E) \sim 1/Q(E)$ or $\lambda(E) = b/Q(E)$, where b is an unknown coefficient of proportionality. The current level of methods solving the tasks of quantum mechanics and experimental techniques allows reliably determining dependence $Q(E)$ for almost any gases [3] (see Figure 1 for N_2 [4]). The mean free path length λ_0 from Eq. (1) was obtained within the classical model for collisions of elastic balls and its value was sustained by experiments. Dependence $Q(E)$ is a result of the quantum-mechanical interaction of an electron with a molecule. Since applicability of the classical physics is always limited by narrow frames in the general quantum-mechanical conception then it is necessary to determine the frames of its applicability in our case. Quantum-mechanical effects of the electron-molecule interaction (e.g. Ramsauer effect) prevail under the energy below than 1-5 eV. If the energy is above 10 eV, ionization of most known atoms and molecules is carried out. So classical and semiclassical models of the "electron - neutral particle" collisions "work" well within the range 1 eV – 10 eV approximately and they allow determining dependence of the scattering cross-section from energy in this case $Q_{classical}(E) \sim 1/\sqrt{E}$ [5]. All above mentioned facts allow evaluating an average value of energy $\bar{E}$ of such range for each gas and obtaining the formula to calculate an unknown coefficient

$\lambda(\bar{E}) \cdot Q(\bar{E}) = \lambda_0 \cdot Q(\bar{E})$. In particular an average energy of the "classical" range is equal to $\bar{E} \approx 3$ eV for nitrogen (Figure 1). The expression for *b* allows determining the desired dependence

$$\lambda_E = \lambda(E) = \lambda_0 \cdot \frac{Q(\bar{E})}{Q(E)} \tag{2}$$

For practice relationship *Q(E)* is to be approximated by the spline function.

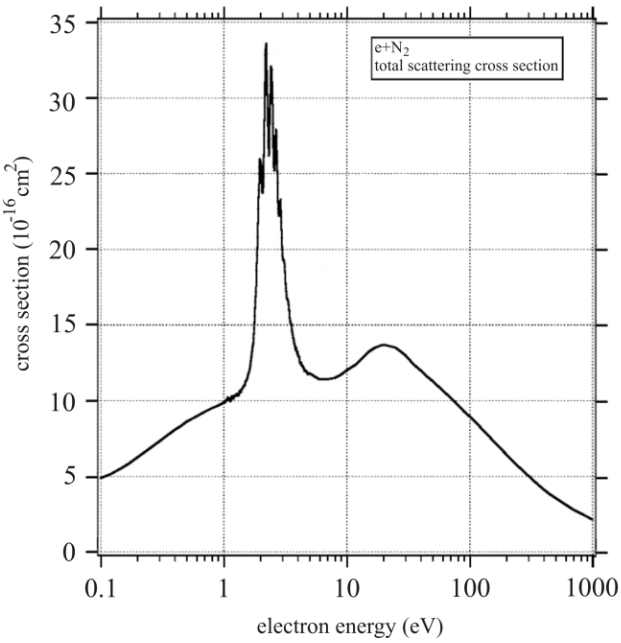

Figure 1. Recommended values of the total scattering cross section *Q(E)* of N_2.

For statistical sampling the length of a free path is considered as a random value distributed within the range (0,∞) with probability density $f(\lambda) = \frac{1}{\lambda_E}\exp(-\frac{\lambda}{\lambda_E})$ [6]. The result of this is a formula of free path length simulation:

$$\lambda = \lambda_E \ln r \tag{3}$$

hereinafter *r* is a specific value of the number distributed uniformly within the interval [0,1] and obtained under the statistical sampling.

Collisions of electrons with molecules can have elastic and inelastic characters. Under the elastic collision there is a change of the motion direction of interacted particles and their speeds. Change of momentum and kinetic energy is carried out but the intrinsic energy of particles remains unchanged. Under the intrinsic collision the intrinsic energy and molecule state are changed.

Probability of the elastic collision is $P_e(E)=Q_e(E)/Q(E)$, probability of the inelastic collision $P_i(E)=Q_i(E)/Q(E)=[1-Q_e(E)]/Q(E)$, because the total scattering cross section *Q* is equal to the amount of cross sections of elastic Q_e and inelastic Q_i interactions: $Q=Q_e+Q_i$. Usage of known dependences of scattering cross sections for each specific gas allows sampling the character of the collision of an electron and molecule according to

$$Collisions = \begin{cases} elastic, 0 \le r \le P_e \\ inelastic, P_e < r \le 1 \end{cases} \tag{4}$$

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In particular the dependences $Q(E)$ (Figure 1) and $Q_e(E)$ recommended in paper [4] allow plotting $P_e(E)=Q_e(E)/Q(E)$ (Figure 2) and implementing the algorithm (4) for collisions of an electron with nitrogen molecules.

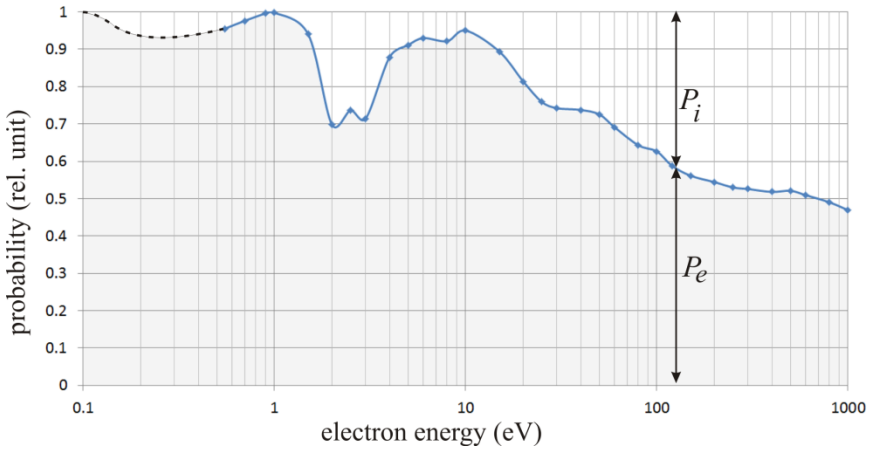

Figure 2. Diagram of the dependence $P_e(E)$ and pattern of the simulation of elastic and inelastic collisions of an electron with N_2 molecules.

Under the elastic interactions the scattering of electrons is carried out without loss of their energy at various angles. Differential scattering cross sections (DCS) of electrons with different energy on nitrogen molecules are researched in papers [7,8]. The analysis of mentioned data allows carrying out piece-smooth patch of the probability density function $f(\varphi)$ of the scattering angles φ under the elastic collisions of electrons in this case (Figure 3). The more accurate approximation is possible only under the greater volume of theoretical and experimental materials.

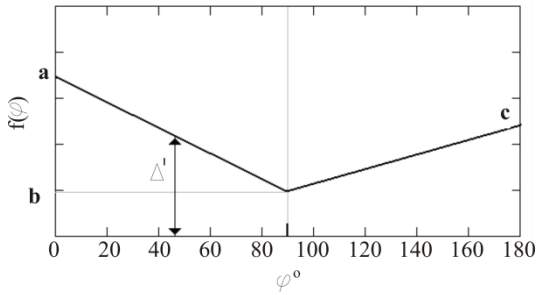

Figure 3. Diagram of the probability density of scattering angles.

The analytical expression for function $f(\varphi)$ will have the following form:

$$f(\varphi)=\Delta'=\begin{cases} a-\dfrac{a-b}{90}\varphi, 0\le\varphi\le 90, \\ c-\dfrac{c-b}{90}(180-\varphi), 90<\varphi\le 180. \end{cases} \quad (5)$$

The data described in papers [7,8] allows evaluating the relative dependence of parameters a and c on energy E of the electron falling upon a molecule N_2: $a(E)/b=E/3$, $c(E)/b=4\text{-}0.4E$. The same dependences we can get to other molecules easily.

Scattering angles can be statistically simulated as discrete quantities, e.g. quantities present at the interval of 1°, according to the following described (standard) pattern.

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Parameter b is considered to be equal to 1. Parameters a and c are calculated for each energy value. Value Δ'_i is calculated for each angle $\varphi_i=i$, i=0.179 according to expression (5). It shall be assumed that $\Delta'_i=0$ for higher energy in the area of angles [90^0, 180^0] if $\Delta'_i<0$. These assumptions correspond to the known fact about decrease of the inverse scattering in proportion to the electron energy increasing. Then normalized quantities (relative values) $\Delta_i = \Delta'_i / \Delta'_\Sigma$ are calculated where $\Delta'_\Sigma = \sum_0^{179} \Delta'_i$. Coordinates of points are calculated as $\xi_{i+1} = \sum_{i=0}^{i} \Delta_i$, i=0…179, while $\xi_0=0$. It should be noted that $\xi_{180}=1$.

It is obvious that scattering probability at the angle φ_i is proportional to the length of a segment Δ_i. Determination of the scattering angle φ_i in each test is carried out according to the condition $\xi_i \le \boldsymbol{r} < \xi_{i+1}$, i=0..179. On the presumption that a scattering angle φ is uniformly distributed within the range $[\varphi_i, \varphi_{i+1}]=1°$, its final value can be calculated as $\varphi=\varphi_i+r$.

Under the inelastic collision an electron transfers a part of its energy to a molecule and changes direction of the original motion. Available testing data [8,9] related to the research of angle dependences of elastic and inelastic collisions can conclude a practical coincidence of angle distributions in the first approximation under the elastic and inelastic interactions of electrons with molecules. That is why the above mentioned technique of simulation of the electron scattering angle under the elastic collision can be applicable to inelastic interactions.

Since an electron under the inelastic interaction with a molecule can transfer a part of its energy in order to initiate rotational transitions (up to tenths of eV), vibrational-rotational transitions (from tenths of eV up to several units of eV), electron-vibrational-rotational transitions (above several units of eV), for ionization (above 10 eV), then it is reasonable to consider a loss of any part of initial electron energy as equally probable under such interaction in the first approximation, or in the following form:

$$E_i = E - \boldsymbol{r}R = E(1-\boldsymbol{r}) = E\boldsymbol{r}$$

where E_i – electron energy after an inelastic interaction.

Under the preset components of the electron speed v_x, v_y and v_z, determining the current direction of the electron speed and defined value of the scattering angle φ (under elastic and inelastic interactions) by means of analytical geometry, directional cosines determining a new direction of the electron motion after scattering can be calculated. It is necessary to introduce an orthogonal basis of vectors $\vec{n}, \vec{q}, \vec{p}$, where a vector $\vec{n}$ is codirectional with the electron speed $\vec{v} = v_x\vec{\imath} + v_y\vec{\jmath} + v_z\vec{k}$ before the collision and determined by directional cosines $\cos\alpha = \frac{v_x}{v}$, $\cos\beta = \frac{v_y}{v}$, $\cos\gamma = \frac{v_z}{v}$, where a speed module is the following $v = \sqrt{{v_x}^2 + {v_y}^2 + {v_z}^2}$. The parameter *mincos*=min[|cos α|,|cos β|,|cos γ|] is determined as follows.

If *mincos*=|cosα|, then the vector $\vec{p}$ has components

$$p_x=0,\ p_y = \frac{\cos\gamma}{\sqrt{\cos^2\gamma + \cos^2\beta}},\ p_z = \frac{\cos\beta}{\sqrt{\cos^2\gamma + \cos^2\beta}}.$$

If *mincos*=|cos β|, then $p_x = \frac{\cos\alpha}{\sqrt{\cos^2\alpha + \cos^2\gamma}}$, $p_y=0$, $p_z = \frac{\cos\beta}{\sqrt{\cos^2\alpha + \cos^2\beta}}$.

If *mincos*=|cos γ|, then $p_x = \frac{\cos\beta}{\sqrt{\cos^2\alpha + \cos^2\beta}}$, $p_y = \frac{\cos\alpha}{\sqrt{\cos^2\alpha + \cos^2\beta}}$, $p_z=0$.

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Components of the vector $\vec{q}$ can be calculated according to the sequence of below mentioned formulas. First it is necessary to determine absolute values of components $q_{0x} = p_z\cos\beta - p_y\cos\gamma$ $q_{0y} = p_x\cos\gamma - p_z\cos\beta$, $q_{0z} = p_y\cos\alpha - p_x\cos\beta$. Then normalized values $q_x = \frac{q_{0x}}{q}, q_y = \frac{q_{0y}}{q}$, $q_z = \frac{q_{0z}}{q}$ are evaluated where a length of the defined vector is $q = \sqrt{q_{0x}^2 + q_{0y}^2 + q_{0z}^2}$.

The scattering angle φ is an angle between vectors $\vec{v}$ and $\vec{u}$. The angle θ specifies orientation of the speed vector $\vec{u}$ in space and it is simulated as a random value distributed uniformly in the range [0,2π], i.e. θ = *r*2π.

As a result new directional cosines $\cos\alpha_u$, $\cos\beta_u$, $\cos\gamma_u$ (after scattering of the electron at the angle φ) are determined according to expressions

$\cos\alpha_0 = \cos\alpha\cos\varphi + \sin\varphi\left[p_x\cos\theta + q_x\sin\theta\right]$, $\cos\beta_0 = \cos\beta\cos\varphi + \sin\varphi\left[p_y\cos\theta + q_y\sin\theta\right]$, $\cos\gamma_0 = \cos\gamma\cos\varphi + \sin\varphi\left[p_z\cos\theta + q_z\sin\theta\right]$, $\cos\alpha_u = \frac{\cos\alpha_0}{s}$, $\cos\beta_u = \frac{\cos\beta_0}{s}$, $\cos\gamma_u = \frac{\cos\gamma_0}{s}$, where $s = \sqrt{\cos^2\alpha_0 + \cos^2\beta_0 + \cos^2\gamma_0}$.

Directional cosines help to find speed components after the electron scattering:

$$u_x = \sqrt{\frac{2E}{m}}\cos\alpha_u,\ u_y = \sqrt{\frac{2E}{m}}\cos\beta_u,\ u_z = \sqrt{\frac{2E}{m}}\cos\gamma_u, \qquad (7)$$

where E is the electron energy after the collision that is equal to energy of the falling electron under the elastic collision and less than this energy under the inelastic collision (E=E_i), m – electron mass.

The pressure *(P)*, gas temperature *(T)* and gas-kinetic molecule diameter *(d)* are set to make calculations of the electron motion under the conditions of interactions. A mean length of a free path λ_0 is determined according to Eq. (1) in the gas-kinetic approximation and a process of the trajectory simulation is started.

Calculation of each segment of the trajectory starts with determination of the electron free path length value λ_E according to the current value of its kinetic energy E according to Eq. (2) and statistical sampling of the specified free path length value λ in the present test in Eq. (3). Then differential equations of electron motions are numerically integrated in the electromagnetic field. Within the calculation under the equality of the trajectory segment length to the free path length λ the collision of an electron with a molecule is considered as happened. Then according to condition (4) character of the collision is determined, elastic or inelastic. For elastic collisions the scattering angle φ (ref. [5]) and the electron speed components according to the final formula (7) are also determined after interaction with a molecule. For inelastic collisions the scattering angle φ (ref. [5]), energy E_i (ref. [6]) and speed components $\vec{u}$ (ref. [7]) of the electron are determined after interaction with a molecule. Then calculations are repeated for the following trajectory segment also.

The qualitative check of the above mentioned model adequacy has been carried out on the experimental mockup consisting of a vacuum diode with a planar cathode and anode. Researches have shown that under letting-to-air consisting of nitrogen in 80%, initial (in vacuum) current was reduced approximately in four times. Calculations according to the mentioned technique also provide such order related to the relative decrease of a number of emitted electrons under their motions.

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Figure 4 demonstrates a results of trajectory analysis of the electron optical system under vacuum (1) and under nitrogen pressure of P = 5 Pa (2). Trajectories are performed in the cylindrical (a) and Cartesian (b) coordinate systems. The accelerating voltage is 100 V. The initial electron energy is 1 eV.

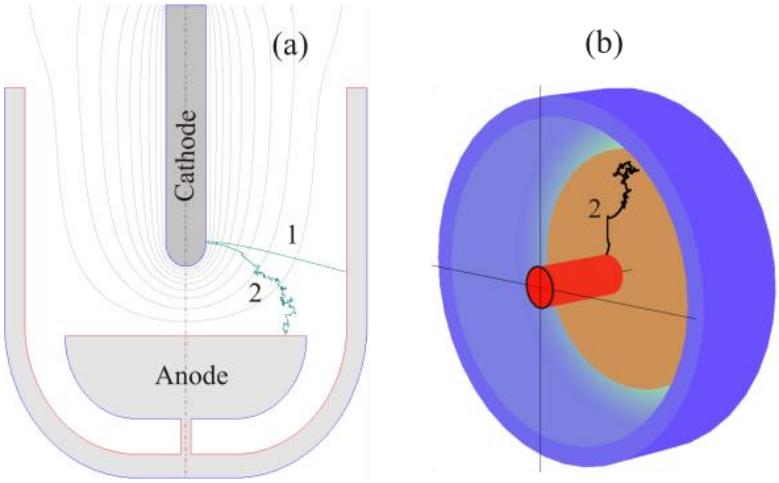

Figure 4. Example of the electron motion in vacuum (1) and nitrogen atmosphere P = 5 Pa (2).

As a conclusion we note that this paper has developed a numerical model of electron motions in the gas media and the qualitative experimental testing of its adequacy for nitrogen has been carried out [10].

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