10.2 Electron beam

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This simulation was made as a solution to one of the International Young Physicist Tournament. Here is a sample problem: An electron beam is cast upon a planparallel of known homogeneous material. Some of the electrons penetrate it, some do not. Try to simulate the processes taking place, e.g. using the Monte Carlo method, and compare your results with those published in the literature.

10.2.1 Introduction

Modeling by the Monte Carlo Method is to simulate with the use of the theory of probability and laws of statistics. This method can be used for solving tasks in which a direct algoritm can not be found, or the algoritm is too complicated to be used in practical solutions. The phenomena that occur during the penetration of electrons in solids are known and described. However when we combine these processes there are some influencing parameters which make the direct approach impossible. In the Monte Carlo Method we use models of simple processes in which we include a certain random factor. When we combine these processes we obtain the complex process which includes the influencing factors. If we make a great numer of these simulations we will get certain output values or their distribution. The more simulation runs we make the more accurate our result will be.

In our simulation we will always trace one (primary) electron, it is to be the so-called single particle model. When we want to simulate the trajectory of the primary electron we have to follow a couple basic steps. The firt thing is to find out the free path which the electron traveled between two consecutive colisions and the final position of the electron. The next step is to determine what kind of collision is taking place, the angle at which the electron was scattered, and the energy loss of the electron. We repeat this algoritm until the energy of the primary electron is lowered to the level on which the electron can be considered absorbed, or until the electron leaves the target. In order to simulate these processes we need to know the total cross-sections, mean free paths of each single process, and the differential cross-sections of the processes; for which we need to know their dependencies on the scattering angle or on the energy loss of the primary electron.

Because the description of the task is too general we have to simplifiing thing a bit. We have decided to simulate electrons that have energy in

the range of hundreds of eV to hundreds of keV. We also suppose that the target is homogeneous and composed of atoms of only one element. We also had to neglect emisions of the secondary electrons,and effects of diffraction. The main objective of our work was to make a simulator that will not be too demanding on the input parameters, but will be able to produce some relatively good results.

10.2.2 Elastic scattering

As we stated earlier an electron is scattered on its way through the target on the atoms of the solid. The collisions that occur can be divided into two groups-elastic and inelastic, by the amount of energy that the electron loses during the collision.

If the electron scatters on the nucleus of the atom we can consider the scattering to be elastic. This also is a certain simplification. We know that in reality there is always some energy loss. However the energy loss is very minimal (about 10^{-2} eV), so we can neglect it and consider the scattering to be elastic.

Because the electron scattering on the nucleus is very localized, this means that the adjacent atoms have no influence on the collision, it's possible to use the model of elastic collision on a single atom as a model of elastic scattering. There are three main models used for simulating the elastic collision on a single atom:

a) Tabulated cross-sections.

b) Rutherford's model.

c) Mott's modiffication of Rutherford's model, which includes the influence of the electron's spin.

The first method gives good results, but it has some disadvantages. There is a need for numerical integration during calculating when we use this method, this would slow down the whole simulation remarkably. Also the data are not available for all elements in all energy ranges. Because of this, we have decided to apply the second method. This method is much easier and it also gives quite good results. The detailed comparison of different ways of modeling elastic scattering can be found in the literature[1].

We will show the formulas for a total cross-section σ and differential cross-section $\frac{d\sigma}{d\Omega}$ for Rutherford's model(Ω is a solid angle). This model includes the influence of the electron cloud on the value of

electric potential V. This potential is then by Wentzel[8]:

$$V = -\frac{e^2 Z}{4\pi\epsilon_o r} e^{-\frac{r}{R}},$$

e is an electron charge,ϵ_o dielectric constant ,and r the distance from the center of the atom. And the radius of atom R is:

$$R = a_H Z^{-\frac{1}{3}},$$

a_H is the Bohr's radius of the atom($a_H = 0.0569nm$). Differential cross-section $\frac{d\sigma}{d\Omega}$ is then by [4] expressed as:

$$\frac{d\sigma}{d\Omega} = \frac{4Z^2}{a_H^2} \frac{(1 + E/E_o)^2}{[(\frac{4\pi}{\lambda_e}\sin\frac{\theta}{2})^2 + \frac{1}{R^2}]^2}, \tag{38}$$

where λ_e is the wave-length of the electron, E is the energy of the electron, E_o is a rest energy of the electron: $E_o = m_o c^2 = 511keV$.

The expression (38) is valid for relativistic electrons. In that case we use an expression for electron's wave length

$$\lambda_e = \frac{h}{\sqrt{2m_o E(1 + \frac{E}{2E_o})}}, \tag{39}$$

where m_o is the rest mass of the electron. In the case of non-relativistic electrons we can set $(1 + E/E_o)^2 = 1$ and $\lambda_e = \frac{h}{\sqrt{2m_o E}}$. Because the angle θ is quite small we can use an aproximation to simplify the problem.We set $\sin\frac{\theta}{2} = \frac{\theta}{2}$. Using this we can simplify the expression(38) into

$$\frac{d\sigma}{d\Omega} = \frac{4Z^2 R^4}{a_H^2} \frac{1}{[1 + (\frac{\theta 2\pi R}{\lambda_e})^2]^2}. \tag{40}$$

the solid angle Ω can be expressed as $d\Omega = \sin\theta\, d\theta\, d\phi$ where θ is a polar angle $(0 < \theta < \pi)$ and ϕ is an azimuth angle $(0 < \phi < 2\pi)$. The value of $\frac{d\sigma}{d\Omega}$ doesn't depend on the value of the azimuth angle ϕ.

We can get the total cross-section σ by integrating the expression(38) over the full solid angle Ω.

$$\sigma = \int_\Omega \frac{d\sigma}{d\Omega} d\Omega = 2\pi \int_0^\pi \frac{d\sigma}{d\Omega} \sin\theta d\theta = \frac{16\pi Z^{\frac{4}{3}}}{(\frac{4\pi}{\lambda_e})^2 + \frac{1}{R^2}} (1 + \frac{E}{E_o})^2 = \frac{16\pi Z^{\frac{4}{3}} R^2}{(\frac{4\pi R}{\lambda_e})^2 + 1}. \tag{41}$$

From this we can derive a formula for probability density of electron scattering with its dependence on the scattering angle θ:

$$f(\theta) = \frac{2\pi \frac{d\sigma}{d\Omega} \sin\theta}{2\pi \int_0^\pi \frac{d\sigma}{d\Omega} \sin\theta d\theta}. \tag{42}$$

the probability p of electron being scattered into an angle α is then

$$p = \int_0^{\alpha} f(\theta) d\theta. \tag{43}$$

After integration

$$p = \frac{(16\pi^2 R^2 + {\lambda_e}^2)(\cos(\alpha) - 1)}{2(8\pi^2 R^2 \cos(\alpha) - 8\pi^2 R^2 - {\lambda_e}^2)}. \tag{44}$$

By manipulating this expression we can easily get a formula for the scattering angle α depending on a random number R_n which ranges from 0 to 1.

$$\alpha = \frac{\pi}{2} - asin[\frac{16\pi^2 R^2(R_n - 1) + {\lambda_e}^2(2R_n - 1)}{16\pi^2 R^2(R_n - 1) - {\lambda_e}^2}]. \tag{45}$$

Formulas (38) and(45) that we derived are dependent only upon the parameters of the target and primary electrons. We can use these formulas to obtain parameters of the electron's trajectories inside the solid. From the total cross-section we are able to get an expression for mean free path (λ) that the electron travels between two elastic collisions.

$$\lambda = \frac{A}{N_a \sigma}, \tag{46}$$

N_a is an Avogadro's number and A is a relative atom number. The mean free path is then measured in terms of mass thickness(kg/m^2). From now on we will measure all distances in terms of mass-thickness, as it is usual in simulations like these.

When the elasting collision occurs we have to find the angle that the electron was scattered into. We get this angle by substituting a random number from the interval $(0, 1)$ for R_n in formula (45).

10.2.3 Inelasting scattering

The inelastic collision is, in comparison to the elastic one, less localized. It means that the adjacent atoms influence the scattering. When the primary electron scatters it looses some energy. In this case the energy loss is not negligible. For simulating the inelastic scattering Bethe's model of continuous slowing down is very often used, as well as a model of a single particle inelastic scattering.

Bethe's model of continuous slowing down When we use the *Bethe's model of continuous slowing down* we consider only elasting collisions. It means that the primary electron can change its direction

only because of the elastic collisions, and the change of its energy depends upon the length of its trajectory between collisions. The amount of lost energy is given by a basic formula

$$\Delta W = \int_{x_1}^{x_2} F dx, \tag{47}$$

where F is a force acting on the electron for which there is Bethe's fomula [4]

$$F = \frac{e^4 N_a Z}{4\pi\epsilon_o^2 A E_o \beta^2} \ln\left(\frac{E_o\beta^2}{2J}\right), \tag{48}$$

where $\beta = v/c$. In the case of nonrelativistic electrons we can make a substitution $E_o\beta^2 = 2E$. It is necessary to mention the variable J which is a mean ionisation potential. The mean ionisation potential was derived by Caldwell[5] as a function of proton number Z

$$\frac{J}{Z} = 12(1 + 0.5Z^{-}1) + 0.03Z.$$

Or shortly $J/Z = 13$. As can be seen the expression(48) is not going to work for low energies because of the logarytmic term(the energy loss becomes negative). There must be some adjustments in order to make a succesful simulation. We can either set the energy, at which we consider the electron to be absorbed, to a value for which the fomula (48) works, or we have to make some adjustments to the mean ionisation potential. In the literature [11] we have found that the mean ionisation potential can be adjusted like this:

$$J = \frac{J_c}{1 + \frac{kJ_c}{E}}, \tag{49}$$

J_c is the original Caldwell's mean ionisation potential and k is aproximately 0.85. This way of simulating is quite simple, however it can give some good results.

Model of single inelastic scattering There is a difference between the previous model of inelasting scattering and this one. In this model the primary electron scatters in two types of collisions-elastic and inelastic ones. The electron doesn't loose its energy during travel, but rather during the inelastic collisions that are simulated separately. In these collisions the electron also changes the direction of its trajectory. In order to create such a model of inelastic scattering we need to know the mean free path λ between two collisions.

$$\lambda = \frac{W_{av}}{F} = \frac{1}{F_b}\int_{W_{min}}^{W^{max}} W f(W) dW, \tag{50}$$

where $W_{av}$is a mean value of the lost energy during the inelastic collision. F is a stopping force acting on the primary electron that slows the electron down. $f(W)$ is a probability density of electron loosing the energy W,and W_{min} and W_{max} are boundary limits of the electron's energy loss. In this model we suppose that

$$\frac{d\sigma_{in}}{dW} = \frac{\pi e_{el}{}^4}{E_o W^2}.$$

The value of the energy loss W can then be expressed as:

$$f(W) = \frac{\frac{d\sigma_{in}}{dW}}{\int_{W_{min}}^{W_{max}} \frac{d\sigma_{in}}{dW} dW} = \frac{W_{min} W_{max}}{W_{max} - W_{min}} W^{-2}. \tag{51}$$

Maximal energy loss W_{max} can be maximally equal to the momental energy of the primary electron E. After subtitution:

$$f(W) = (\frac{EW_{min}}{E - W_{min}}) W^{-2}. \tag{52}$$

After substituting to the equation (50) and integration we get:

$$\lambda = \frac{1}{F} \frac{EW_{min}}{E - W_{min}} \ln (\frac{E}{W_{min}}). \tag{53}$$

Minimal energy loss W_{min} is a varying parameter that, when we consider the properties of the function, must be greater than 0. In our simulation it was sufficient to set $W_{min} = 10eV$. From this equation we can finally count the electron's mean free path between two inelastic collisions λ depending on the input parameters and the instantaneous energy of the primary electron. Another thing we need to know is the dependence of the value of the lost energy on a random number. The probability p of the electron losing energy ΔW is

$$p(\Delta W) = \int_{W_{min}}^{\Delta W} f(W) dW = \frac{E(\Delta W - W_{min})}{\Delta W (E - W_{min})}. \tag{54}$$

The energy loss ΔW is then dependent upon the random number R_n:

$$\Delta W = \frac{EW_{min}}{R_n W_{min} - E(R_n - 1)}. \tag{55}$$

The energy loss corresponds to a scattering angle θ: $sin^2\theta = \frac{\Delta W}{E}$. During the simualtion the actual energy loss is obtained from equation(53). All shown calcuations for elastic and inelastic scattering are for the scattering angle θ. The azimuth angle ψ is easily obtained from the formula

$$\psi = 2\pi R_n.$$

10.2.4 Program details

Now we know the mean free paths for both types of collisions, from them we can calculate the electron's total mean free path λ_t:

$$\frac{1}{\lambda_t} = \frac{1}{\lambda_{elast}} + \frac{1}{\lambda_{inel}}.$$

Other important formulas are those used for calculating the position and speed of the primary electron. Let x_n, y_n, z_n be the electron's coordinates after the n-th collision and Θ_n, Ψ_n are the directional and azimuth angle. Let Θ, Ψ are the angles we obtained from the previously shown formulas. For calculating the change of primary electron's direction after every collision (Θ_n, Ψ_n) from the previous direction we use formulas:

$$\begin{aligned}
\cos\Theta_n &= \cos\Theta_{n-1}\cos\Theta - \sin\Theta_{n-1}\sin\Theta\sin\Psi, \\
\sin\Theta_n &= \sqrt{1-\cos^2\Theta_n}, \\
\cos\Psi_n &= \frac{\sin\Psi_{n-1}(\cos\Theta_{n-1}\sin\Theta\sin\Psi + \cos\Theta\sin\Theta_{n-1}) + \cos\Psi_{n-1}\sin\Theta\cos}{sin\Theta_n} \\
\sin\Psi_n &= \frac{\cos\Psi_{n-1}(\cos\Theta_{n-1}\sin\Theta\sin\Psi + \cos\Theta\sin\Theta_{n-1}) - \sin\Psi_{n-1}\sin\Theta\cos}{sin\Theta_n}
\end{aligned}$$

From the new angles Θ_n and Ψ_n, old coordinates x_n, y_n, z_n and the free path δS_n we get new coordinates of the primary electron:

$$\begin{aligned}
x_{n+1} &= x_n + \Delta S_n \sin\Theta_n \cos\Psi_n, \\
y_{n+1} &= y_n + \Delta S_n \sin\Theta_n \sin\Psi_n, \\
z_{n+1} &= z_n + \Delta S_n \cos\Theta_n.
\end{aligned}$$

The first step in our simulation is to find the free pathλ_t as shown above. The next step is to get new coordinates of the primary electron. If the electron is still inside the plate we have to find out, in the next step, what kind of collision is taking place. If

$$R_n \leq \frac{\frac{1}{\lambda_{elast}}}{\frac{1}{\lambda_t}},$$

(can be written as:)

$$R_n \leq \frac{\sigma_{elast}}{\sigma_t},$$

it is an elastic collision. In the other case it will be an inelastic collision (in the single inelasting scattering model). In the case of the inelastic scattering model we have to determine the amount of lost

energy due to the collision. If the primary electron's energy drops below a certain low level the movement of the electron becomes very localized, we can thus consider the primary electron being absorbed. We set this minimal level $E_{min} = 200eV$. If we a used lower energy level the simulation would slow down remarkably, and lowering the minimal energy wouldn't have much influence on the result. In both types of collisions we have to determine the scattering and azimuth angle.

10.2.5 Results

The first thing we focused our simulation on were coefficients of backscattering for thin films. The results of this simulation are mainly influenced by the model of elastic scattering, so these simulations are good for testing the model of elasting scattering(in our case it's a Rutherford's model). We simulated electrons with energy of $50keV$ going through a plate made of aluminium and carbon(pic. 1). For comparison we have decided to show results from the work of V. Starý[1](obr. 2).

Although the description of the task is said to simulate the electron's penetration through a planparallel plate, we decided to simulate the next penetration through a semi-infinite solid. From these simulations we are able to find the mean depth of penetration x in the material(Al, Be, Cu). We carried out these simulations for both types of models of inelasting scattering (Bethe's model and single inelastic scattering model). The obtained results can be seen in pictures 2a and 2b. For comparison we show the results of experiments(pic. 2c) published in[7]. As you can see from the pictures we obtained quite good results for berilium and aluminium. However the results for copper and especially for gold are not that good.

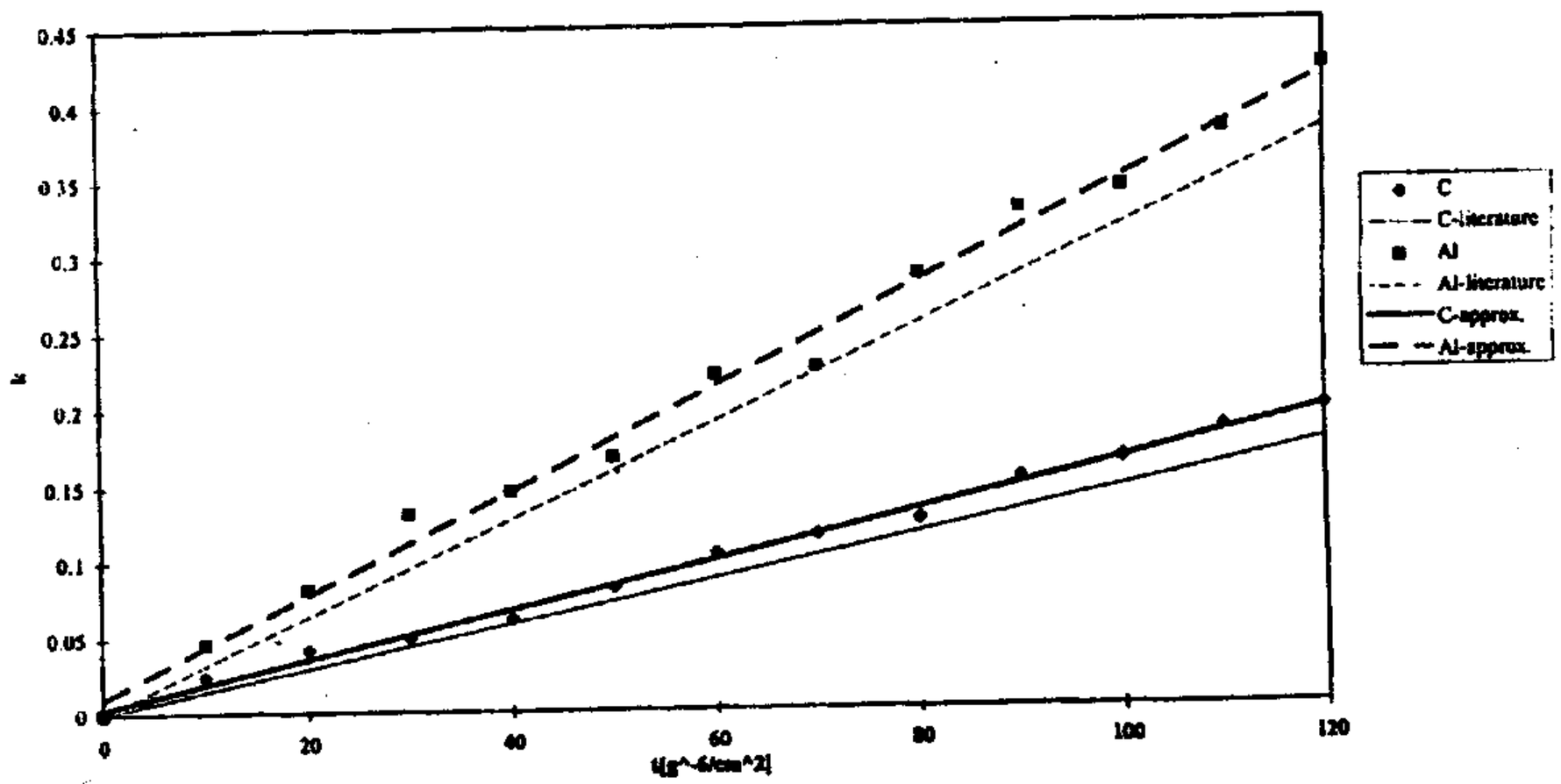
The last thing we simulated were $10keV$ electrons going though a planparallel plate made of copper. In this simulation we were looking for the number of electrons that went through, backscattered or were absorbed(pic. 3a). For comparison we show data from a similar simulation published in[5](pic 3b). Although our simulator doesn't work as well for copper as it does for the other elements we chose this simulation mainly because we had data from literature to compare our results with.

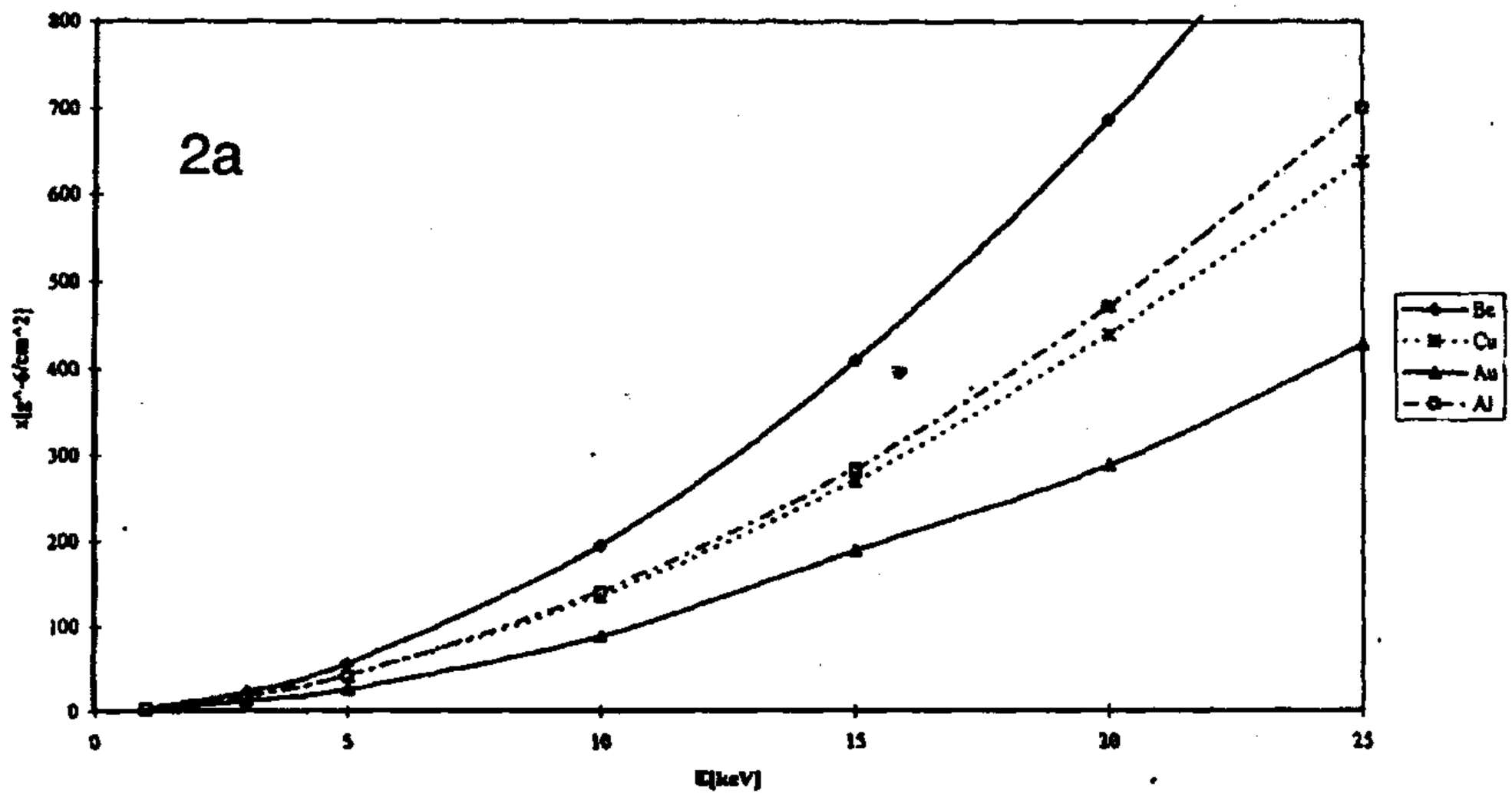
The last picture(num. 4) shows the electron trajectories calculated in a previous simulation. A beam of electrons at energy of 10 keV is cast upon a planparallel copper plate (in the place where the arrow

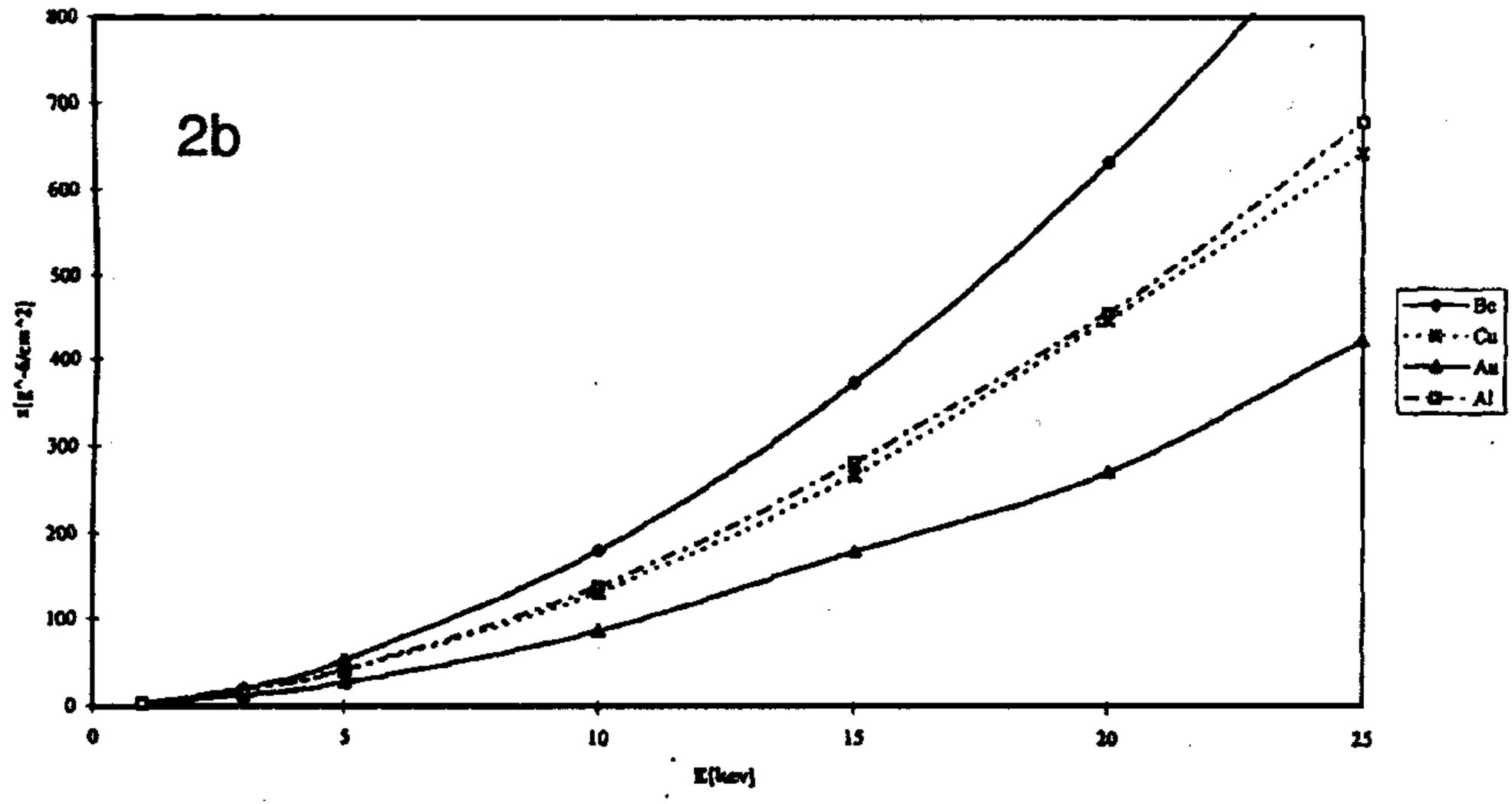
points), which is $250g^{-6}/cm^2$ thick. It can easily be seen from the picture how the electrons scatter in the material and how some of them leave the plate.

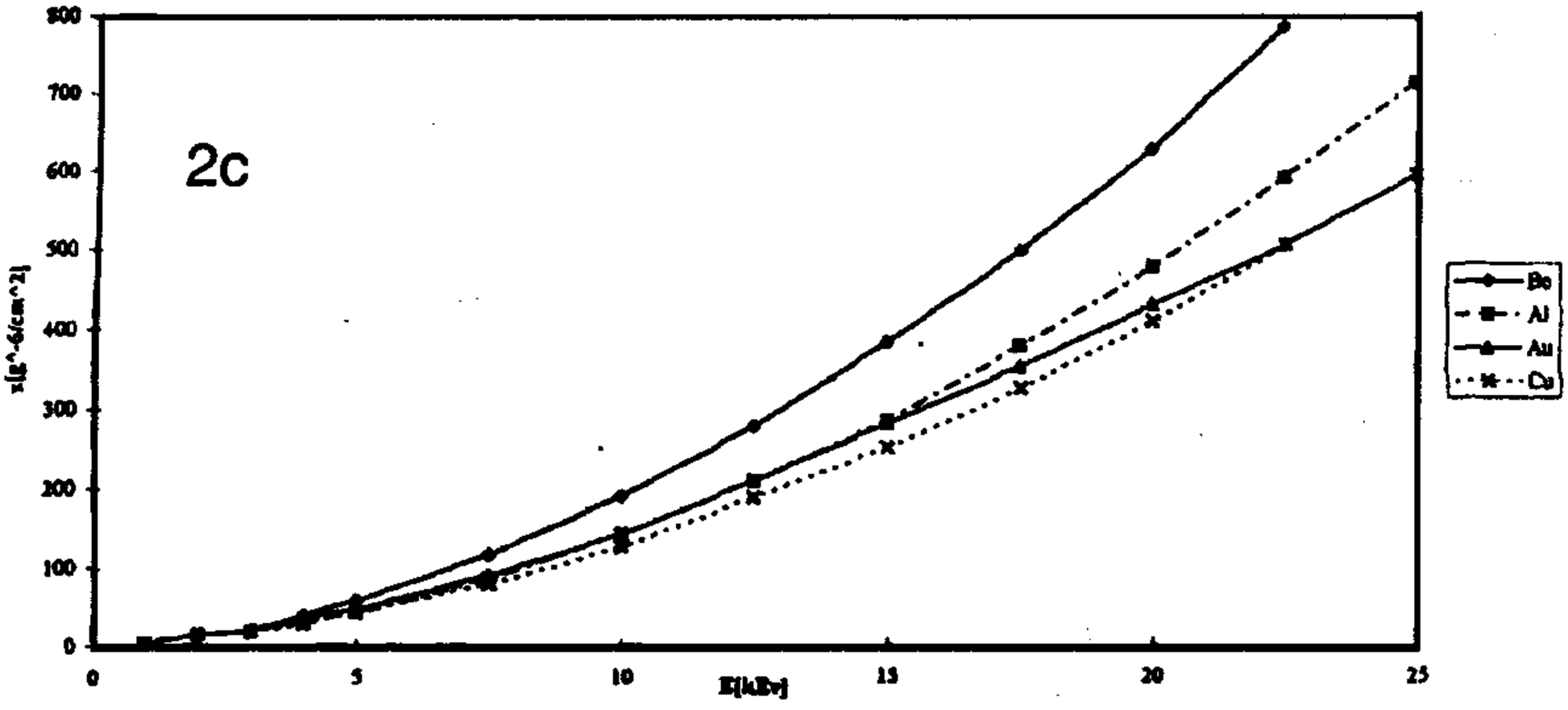
We carried out simulations mainly for aluminium,berilium and copper. We chose these because we were able to compare our result with results published in literature. Although our simulator is very simple and we made lot of simplifications, it gives some results that can be compared with those published in literature.

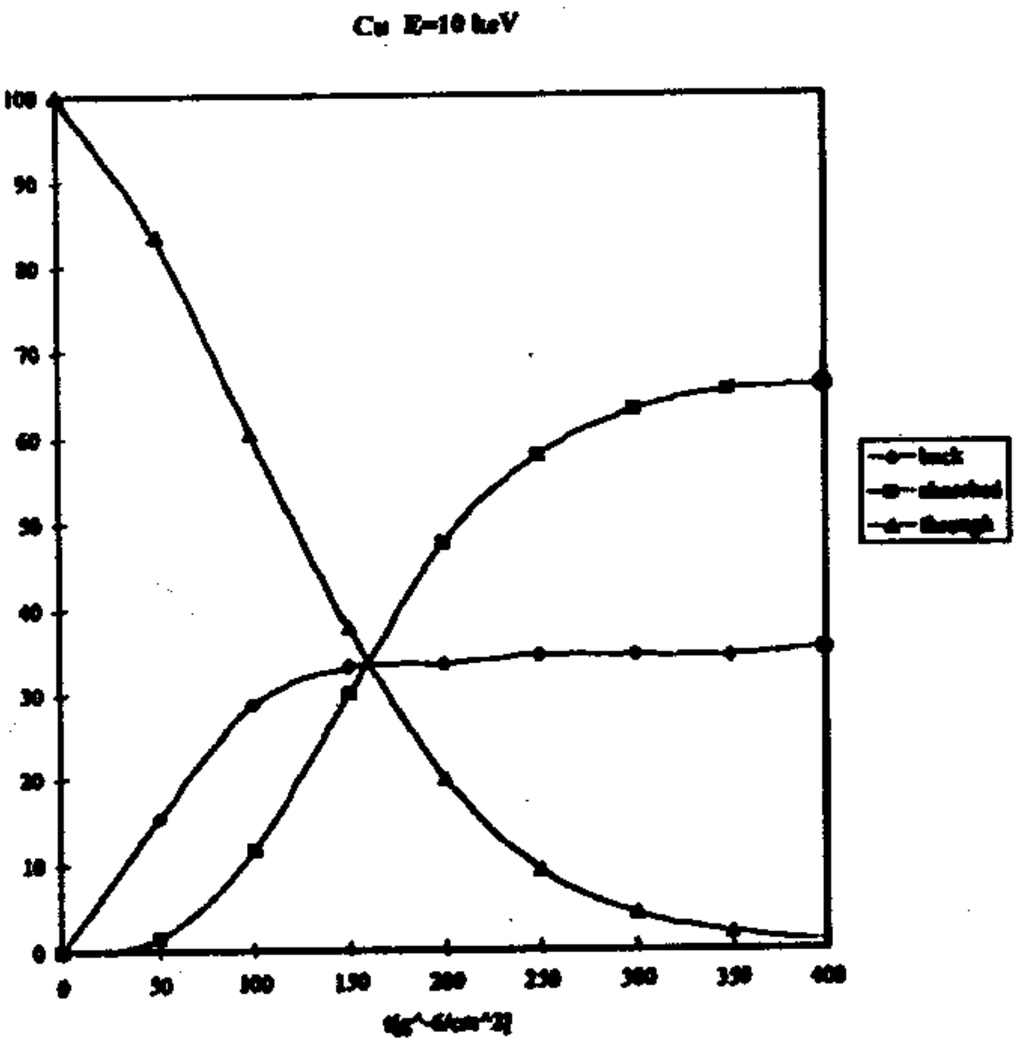
fig. 1

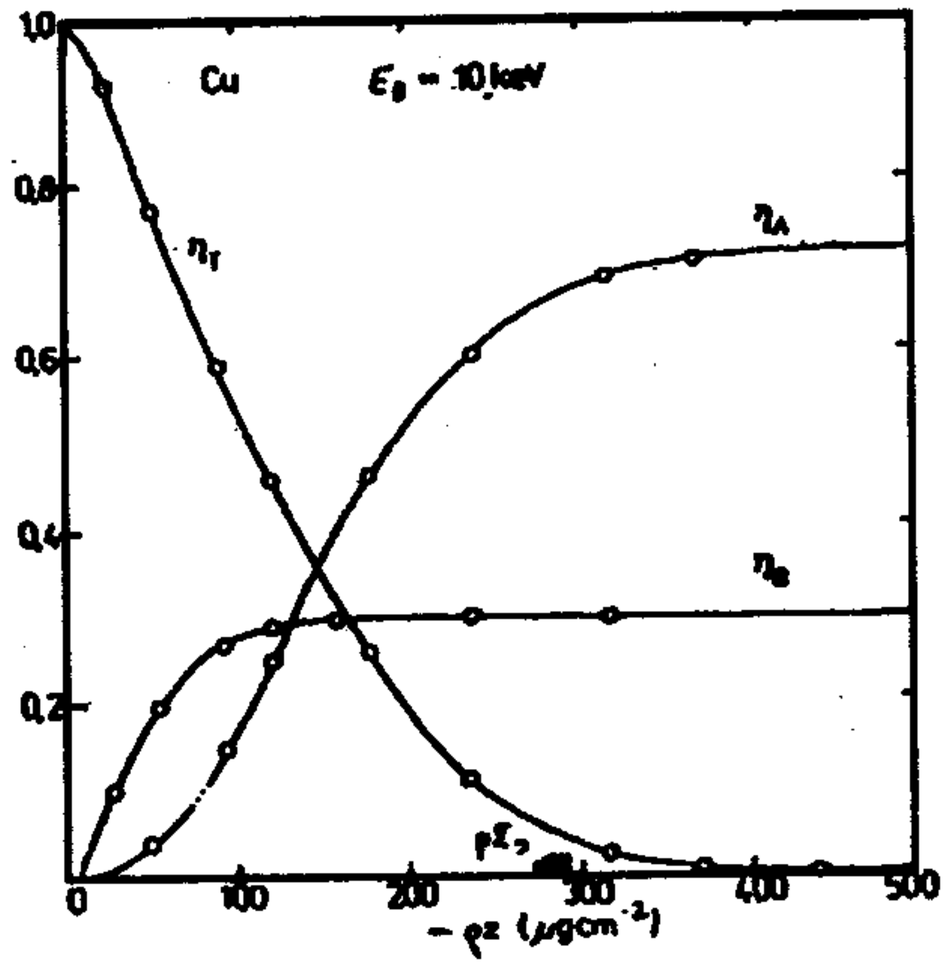


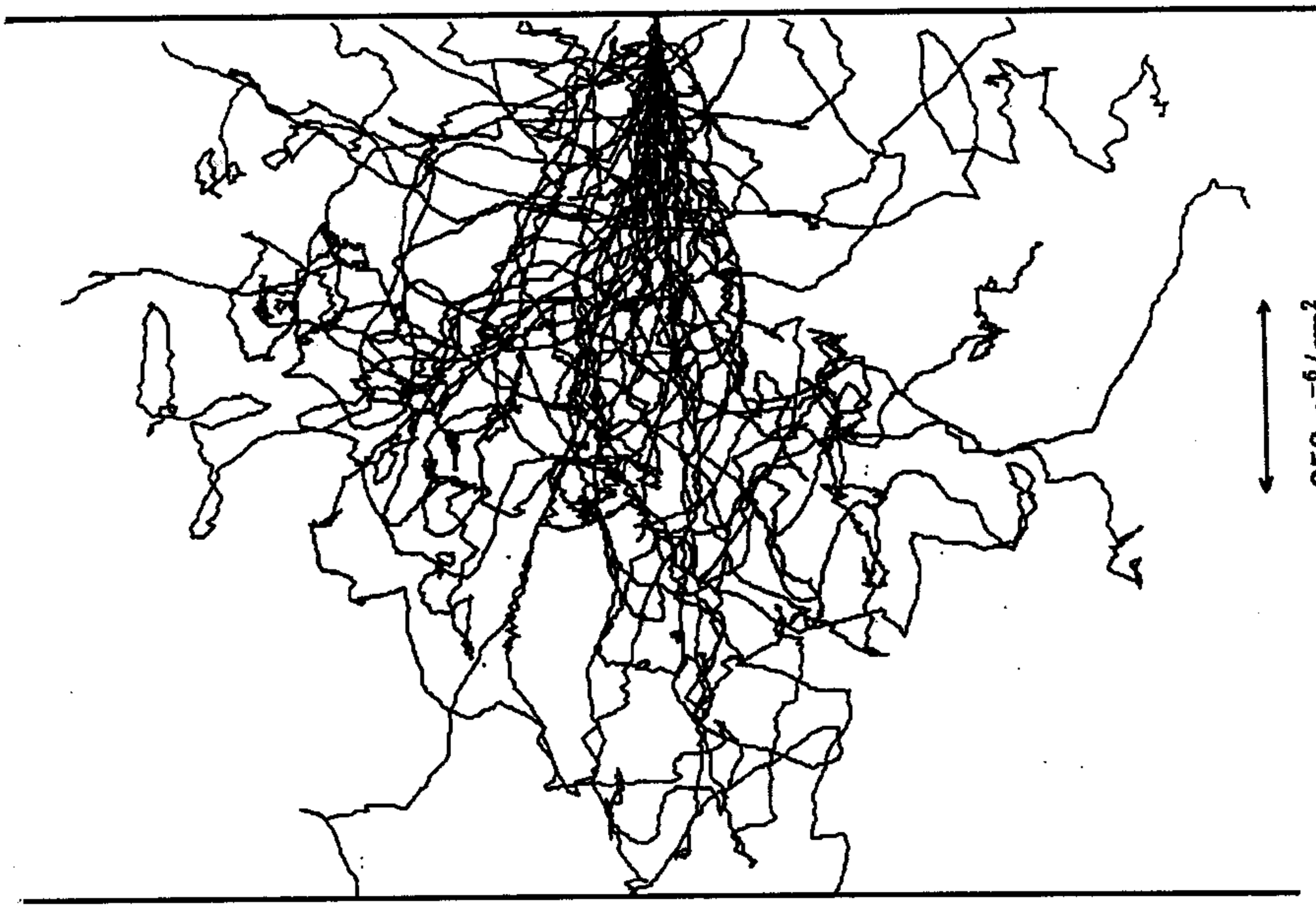

2a
800
700
600
500
400
300
200
100
0
0
5
10
15
20
25
E[keV]
Be
Cu
Au
Al


2b
800
700
600
500
400
300
200
100
0
0
5
10
15
20
25
E[kev]
Be
Cu
Au
Al


2c
800
700
600
500
400
300
200
100
0
0
5
10
15
20
25
E[kEv]
Be
Al
Au
Cu


Cu E=10 keV
100
90
80
70
60
50
40
30
20
10
0
0
50
100
150
200
250
300
350
400


Cu
E_0 = 10 keV
1,0
0,8
0,6
0,4
0,2
η_F
η_A
η_B
$F\Sigma_2$
0
100
200
300
400
500
$-\rho z$ ($\mu g cm^{-2}$)


250 g^{-6}/cm^2

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10.3 Description of pictures

1:
pic.1 Coeficients of backscattering for thin films of C,Al. The results are lineary approximated by thick lines. The thin lines show results taken from literature.

2:
pic.2 Mean depth of penetration of the electron's in Be,Cu,Au,Al and their dependence on electron's energy; a- with a use of model

of continuous slowing down, b- single inelasting scattering model, c- experimental results taken from literature.

3:

pic.3 Number of 10keV electrons that we backscattered, absorbed or went through a planparallel plate made of copper, a- results of our simulation(using the continuous slowing down model) , b- results taken from literature.

4:

pic.4 Trajectories of electron's with the energy of 10keV going through a copper plate of thickness $250g^{-6}/cm^2$