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Simple Monte Carlo Computer Procedure for the Depth Parameters Determination of Implanted Ions in Amphous Targets

Prosta metoda Monte-Carlo określania parametrów rozkładu implatowanych jonów w amorficznych tarczach

Модифицированный метод Монте-Карло для определения параметров распределения имплантированных ионов в аморфные мишени

INTRODUCTION

The Monte Carlo simulation of the slowing down of energetic ions in solids is now widely used in studies of ion implantation, radiation damage and sputtering. It allows more rigorous treatment of the depth profiles of implanted ions giving all required higher moments of the distribution after simple evaluation. This is rather difficult when the present analytical formulation based on transport theory is used. The major inconvenience of the Monte Carlo method is that it requires large computer-time usage, especially for high energy ions

treatment with suitable statistical precision. Each simplification of the method reducing the computer time consumption is then important.

There are several ion transport procedures based on the computer simulation of the slowing down of energetic ions in solids [1 - 11] . One of their major differences lies in the treatment of the nuclear scattering. For example, Robinson et al. [2 - 4] treat this scattering by numerically evaluating classical scattering integral. Other authors used the momentum approximation extended to large angles [5, 6, 10] or truncated Coulomb potential [7 - 9] . Biersack and Haggmark [11] base their formalism on a simple but precise analytical expression for determining nuclear scattering angles for Molier potential /TRIM - program/. The TRIM program reduces computer usage by at least an order of magnitude in comparision with procedures based on the precise numerically treated classical scattering integrals.

In the paper we propose the Monte Carlo procedure based on an alternative analytical method of evaluation of the nuclear scattering angles for the Molier potential. The program reduces significantly computer time consumption also in comparision with fast TRIM procedure keeping up nearly the same accurancy of evaluation.

1. NUCLEAR AND ELECTRONIC ENERGY LOSS EVALUATION

During the slowing down of energetic ions in solids, the particle undergoes many collisions gradually losing the energy as a result of elastic /nuclear/ and inelastic /electronic/ interaction with target's atoms. The nuclear energy loss in a single collision can be easily calculated when scattering angle of the projectile is known. Last one can be treated from clasical scattering integral

$$\theta = \pi - 2b \int_{R_0}^{\infty} \frac{dr}{r^2 \sqrt{1 - \frac{b^2}{r^2} - \frac{V(r)}{E_r}}}$$

where b is the impact parameter, E_r is the relative kinetic energy, r is the interatomic separation, V(r) is the potential of interatomic force, and R_0 is the apsis of the collision defined by $\left(1 - b^2/R_0^2 - \frac{V(R_0)}{E_r}\right) = 0$.

The scattering angle can be also evaluated from approximation analytic formula for example proposed by Biersack and Haggmark [11] .

In this program we use the analytic equation of scattering angle evaluated from Lindhard's [12] nuclear differential cross section of the form

$$d\sigma = \pi/n \left[B^2 a^{2n-2} k_n^2 \beta_n T_m\right]^{1/n} \frac{dT}{T^{(1+1/n)}} \qquad (1)$$

where B is the Bohr's collision diameter, a is the screening length, k_n is a constant, T the energy transfer in the collision,

$$T_m = 4 \frac{M_1 M_2}{(M_1 + M_2)} E = \gamma E$$

$$\beta_n = \frac{3n-1}{8n^2}$$

M_1 and M_2 are the masses of the projectile and target atom respectively, E the initial kinetic energy of the projectile and n is the parameter of the inverse power potential [13] .

By the integration of equation (1) the energy transfer in the collision can be evaluated as

$$T = \gamma E \left\{1 + \frac{b^2 E^{2/n}}{\left[A_0^2 a^{2n-2} \beta_n k_n^2\right]^{1/n}}\right\}^{-n}$$

where b is the impact parameter, and

$$A_0 = 1.4397 \cdot 10^{-7} \frac{M_1 + M_2}{M_2} Z_1 Z_2 \quad [eV, cm]$$

On the other hand

$$T = T_m \sin^2 \frac{\theta}{2}$$

and

$$\sin^2\frac{\theta}{2} = \left\{ 1 + \frac{p^2\,\varepsilon^{2/n}}{[k_n^2\,\beta_n]^{1/n}} \right\}^{-n}$$

or

$$\sin^2\frac{\theta}{2} = \left\{ 1 + \frac{p^2\,\varepsilon^{2/n}}{[\bar{K}_n^2\,\beta_n]^{1/n}} \right\}^{-n}$$

where K_n is a new constant

$P = b/a$ is the reduced impact parameter

$\beta_n = \frac{8n-1}{n^2}$

and $\varepsilon = 6.9456 \cdot 10^6\, a\, \frac{M_2}{M_1+M_2}\, \frac{E}{Z_1 \cdot Z_2}$ [eV, cm]

is the reduced energy.

In the calculation, we have chosen to use the Firsov screening length given by

$$a = \frac{0.8853 a_0}{(Z_1^{1/2} + Z_2^{1/2})^{2/3}}$$

where $a_0 = 0{,}529$ Å is the Bohr radius.

In the equation /2/ parameter n = 1 corresponds to Rutherford scattering n = 2 to weak screening collision and n = 5 to hard sphere collision. In the Monte Carlo simulation method equation /2/ cannot be directly used /with constant value of n and K_n/ because each "history" of an ion begins with high energy and particle undergoes many collisions before it stops.

The n as a function of ε and K_n as a function of P and ε / from the fitting to the Molier potential [14] / can be represented by the following expressions

$$n(\varepsilon) = 1 + 4 \exp(-1.9 \cdot \varepsilon^{0.1}) \qquad (3)$$

and

$$\bar{K}_n = A - D \cdot P - C \qquad (4)$$

where

$$A = 0.224\,[1 + 0.52 \ln(1 + \varepsilon^{1.2})]\, n^{1.206} \sin\left(\frac{n^{2.8}}{13.8 + 0.12\sqrt{\varepsilon}}\right)$$

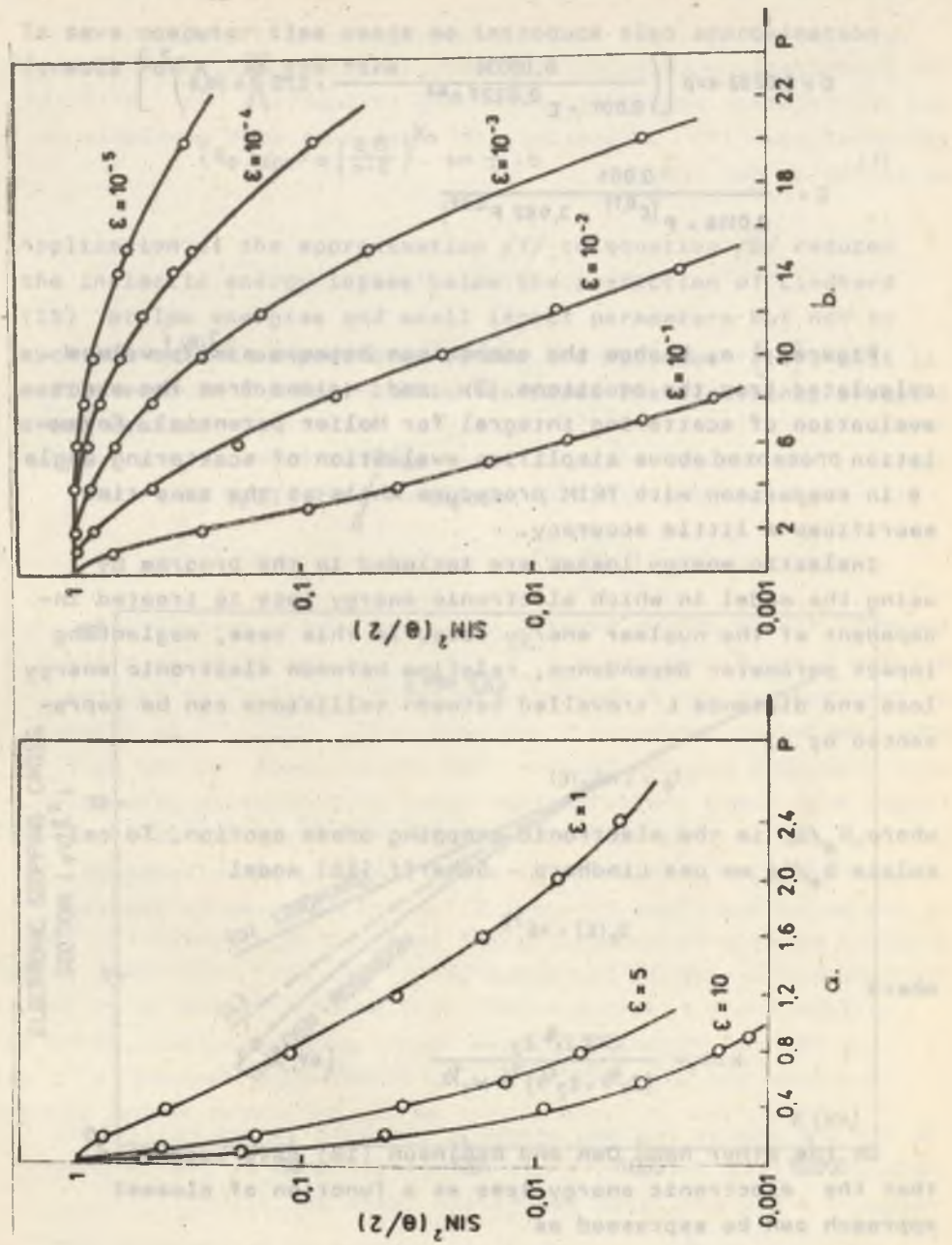

Fig. 1. $\sin^2(\theta/2)$ as a function of reduced impact parameter P for reduced energy between 10^{-5} and 10

$$D = 0{,}0283 \exp\left[\left(\frac{0.00034}{0{,}001 + \varepsilon^{0{,}0227\, n^{3.6}}} + 0{,}75\right)\left(n - 2{,}9\right)^2\right]$$

$$C = \frac{0.001}{0{,}0156 + P^{\left(\varepsilon^{0{,}11} + 3{,}962\, P^{0.82}\right)}}$$

Figures 1 a, b show the comparison between $\sin^2(\Theta/2)$ values calculated from the equations (3) and (4) and from the exact evaluation of scattering integral for Molier potential. Formulation presented above simplifies evaluation of scattering angle Θ in comparison with TRIM procedure while at the same time sacrifices a little accuracy.

Inelastic energy losses are included in the program by using the model in which electronic energy loss is treated indepedent of the nuclear energy loss. In this case, neglecting impact parameter dependence, relation between electronic energy loss and distance L travelled between collisions can be represented by

$$T_e = L N S_e(E)$$

where $S_e/E/$ is the electronic stopping cross section. To calculate $S_e/E/$ we use Lindhard - Scharff [15] model

$$S_e(E) = kE^{1/2}$$

where

$$k = k_l = \frac{1{,}212\, Z_1^{7/6}\, Z_2}{\left(Z_1^{2/3} + Z_2^{2/3}\right)^{3/2} M_1^{1/2}} \qquad [eV, Å^2]$$

On the other hand Oen and Robinson [16] have suggested, that the electronic energy loss as a function of closest approach can be expressed as

$$T_e = \frac{0{,}045k\sqrt{E}}{\pi a^2}\, e^{-0{,}3\, R_0/a} \qquad (6)$$

To save computer time usage we introduce also approximation formula for R_o in the form

$$[R_o]_{app} = a\left(\frac{0,15}{n\cdot\varepsilon}\right)^{1/n} \sin\frac{\theta}{2} + b \qquad (7)$$

Application of the approximation /7/ to equation /6/ reduces the inelastic energy losses below the prediction of Lindhard [15] at low energies and small impact parameters but not to such and extent as predicted by Oen and Robinson [16]. This is easily seen in the Fig. 2 which compares the electronic stopping cross section

$$S_e(E) = 2\pi\int_0^{b_{max}} bT_e\,db$$

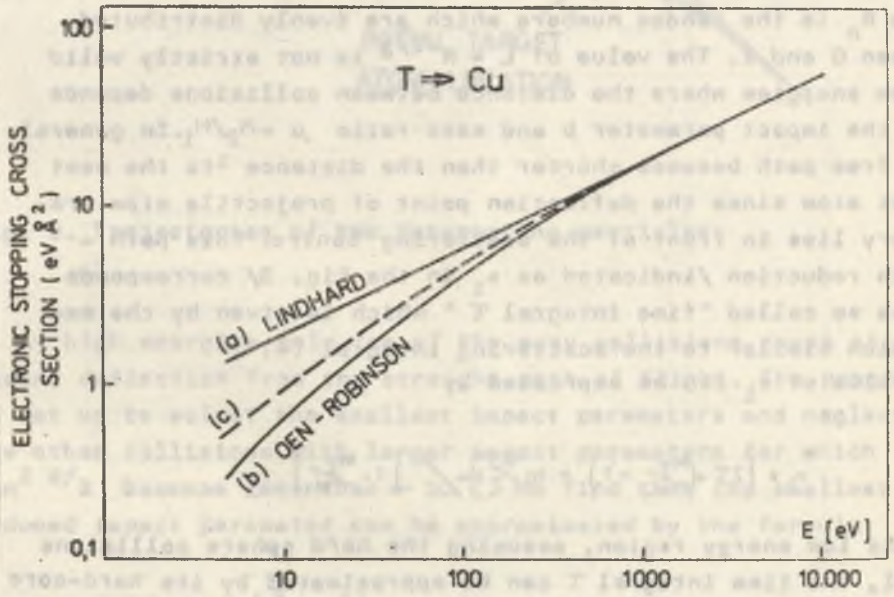

Fig. 2. Electronic stopping cross sections for T incident on Cu in different approximations. Curve /c/ - according to equation /6/ with the approximation /7/

for T incident on Cu calculated according to the Lindhard-Scharff and Oen-Robinson models and according to equation (6) with the approximation (7) . Equation (6) has been made available as an option in our program.

2. DISTANCE BETWEEN COLLISIONS

The targets were assumed to be amorphous, so that the distance between collisions L can be assumed as equal to the mean atomic separation $L = N^{-1/3}$ where N is the atomic density of the target. This assumption leads /according to Biersack and Haggmark [11] / to the determination of impact parameters

$$b = [R_n / (\pi N^{2/3})]^{1/2}$$

where R_n is the random numbers which are evenly distributed between 0 and 1. The value of $L = N^{-1/3}$ is not strictly valid at low energies where the distance between collisions depends upon the impact parameter b and mass ratio $\mu = M_2/M_1$. In general mean free path becomes shorter than the distance ^{1}to the next target atom since the deflection point of projectile atom trajectory lies in front of the scattering centre. This path - length reduction /indicated as x_1 in the Fig. 3/ corresponds to the so called "time integral τ " which is given by the expression similar to the scattering integral [4] .
The value of x_1 can be expressed by

$$x_1 = \left[2\tau + \left(\frac{M_2}{M_1} - 1\right) b \operatorname{tg}\frac{\theta}{2}\right] \Big/ \left[1 + \frac{M_2}{M_1}\right]$$

In the low energy region, assuming the hard sphere collisions model, the time integral τ can be approximated by its hard-core value, $\tau = b \operatorname{tg} \theta/2$. Such assumption leads to

$$x_1 = b \operatorname{tg}\frac{\theta}{2}$$

and

$$L = N^{-\frac{1}{3}} - b \operatorname{tg}(\theta/2)$$

The procedure presented above has been used by Biersack and Haggmark [11] in the TRIM program and is also adopted in this work.

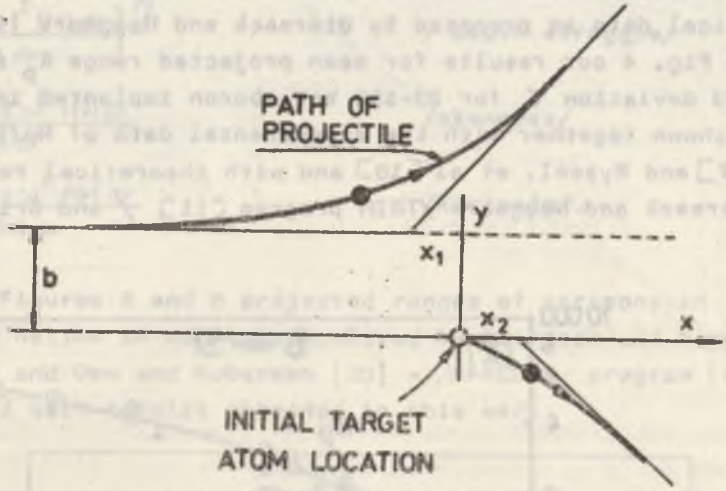

Fig. 3. Trajectories of two interacting particles

At high energies only few of the many collisions cause significant deflection from the straight path of flight. The program is set up to select the smallest impact parameters and neglect the other collisions with larger impact parameters for which $\sin^2 \theta/2$ becomes less then $\sim 10^{-4}$. We find that the smallest reduced impact parameter can be approximated by the formula

$$P_{min} = \left(\frac{6}{\varepsilon^{0.3}} - 1\right) \qquad \text{for } \varepsilon < 400$$

For the parameters larger than P_{min} scattering angles of projectile θ and nuclear energy loss T_n are assumed to 0 and only electronic energy loss is taken into account.

3. RESULTS AND COMPARISIONS

To test the extremely simplified computational technique presented here we use the same set of experimental and theoretical data as proposed by Biersack and Haggmark [11] . In the Fig. 4 our results for mean projected range R_p and standard deviation σ for 20-180 keV boron implanted into silicon is shown together with the experimental data of Hofker et al [17] and Ryssel. et al [18] and with theoretical results of Biersack and Haggmark /TRIM program [11] / and Brice [19].

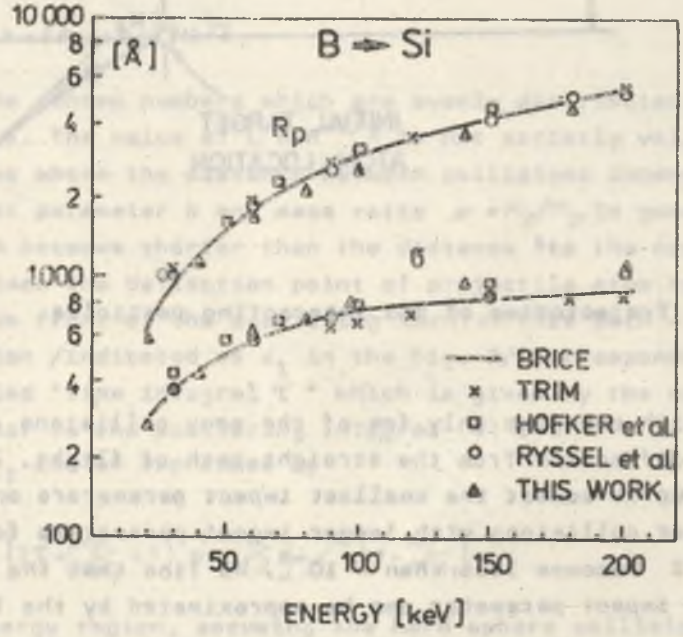

Fig. 4. Mean projected range R_p and standard deviation σ for boron implanted into silicon /□ - experimental data of Hofker at al.[17], ○ - experimental data of Ryssel et al. [18] , — — Brice [19] - $k/k_L = 1.59$, x- TRIM - $k/k_L = 1.59$, ▲ - this work $k/k_L = 1.59$/

The follwing definitions have been used for moments calculations from the Monte Carlo histograms

$$\langle x \rangle = R_p = \frac{\int x\, f(x)\, dx}{\int f(x)\, dx} \qquad \text{/mean projected range/}$$

$$\sigma = \left[\frac{\int (x - \langle x \rangle)^2 f(x)\, dx}{\int f(x)\, dx}\right]^{1/2} \qquad \text{/ depth straggle/}$$

$$S = \frac{1}{\sigma^3} \frac{\int (x - \langle x \rangle)^3 f(x)\, dx}{\int f(x)\, dx} \qquad \text{/skewness/}$$

$$k = \frac{1}{\sigma^4} \frac{\int (x - \langle x \rangle)^4 f(x)\, dx}{\int f(x)\, dx} \qquad \text{/kurtosis/.}$$

In the Figures 5 and 6 projected ranges of antimony in silicon and helium in copper calculated by Biersack and Haggmark /TRIM/ and Oen and Robinson [20] - /MARLOWE program [4] / are compared with results obtained in this work.

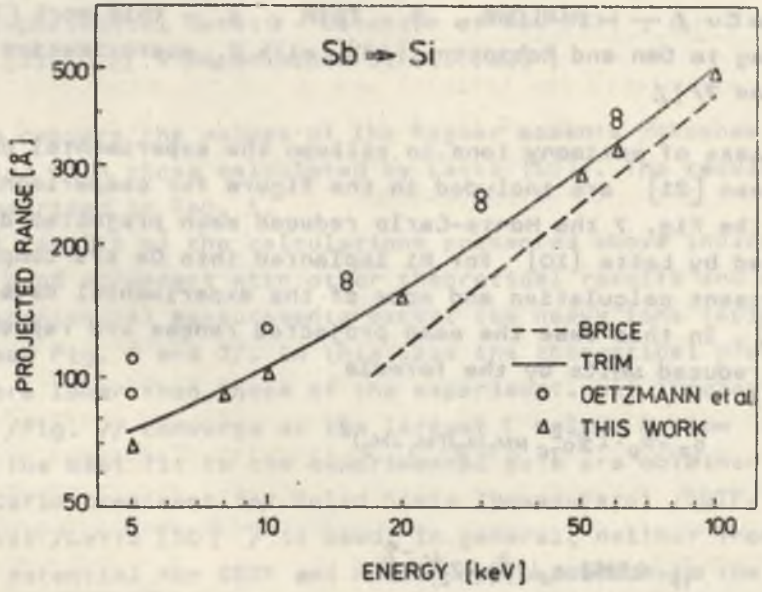

Fig. 5. Projected ranges of Sb ions in silicon /○ - experimental data od Oetzman et al. [21] , — — TRIM results [11] , Δ - this work/

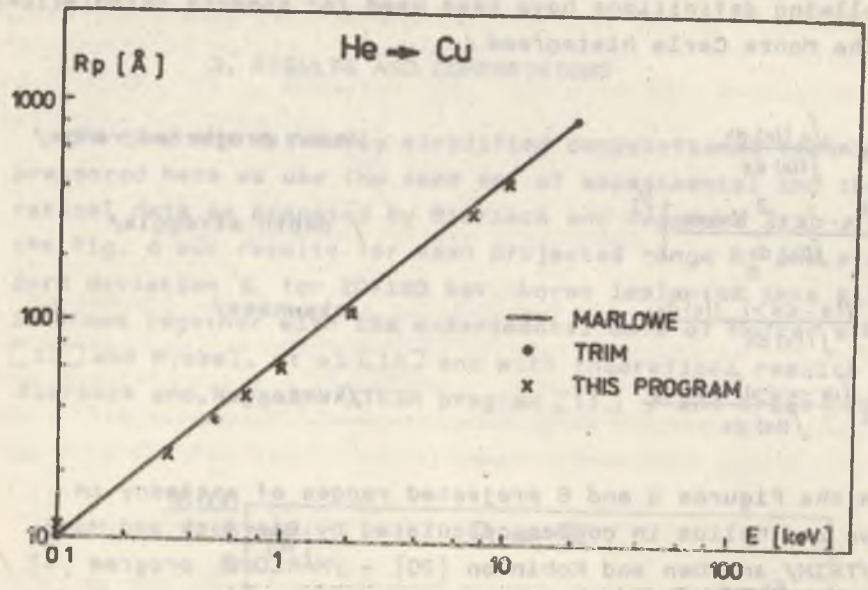

Fig. 6. Mean projected ranges of low energy helium ions implanted into Cu / — = MARLOWE , ● = TRIM , x = this work (T_e = according to Oen and Robinson [16] with R_p approximation /equation 7/)/.

In the case of antimony ions in silicon the experimental data of of Oetzman [21] are included in the figure for comparison.

In the Fig. 7 the Monte-Carlo reduced mean projected depths estimated by Latta [10] for Bi implanted into Ge are compared with present calculation and some of the experimental data [21, 22, 23]. In this case the mean projected ranges are represented in reduced units by the formula

$$\varrho_p = R_p \cdot 4\pi a_{TF}^2 NM_1M_2/(M_1+M_2)^2$$

where

$$a_{TF} = 0.8853 \cdot a_0 (Z_1^{2/3} + Z_2^{2/3})^{-1/2}$$

and $a = 0{,}529$ Å

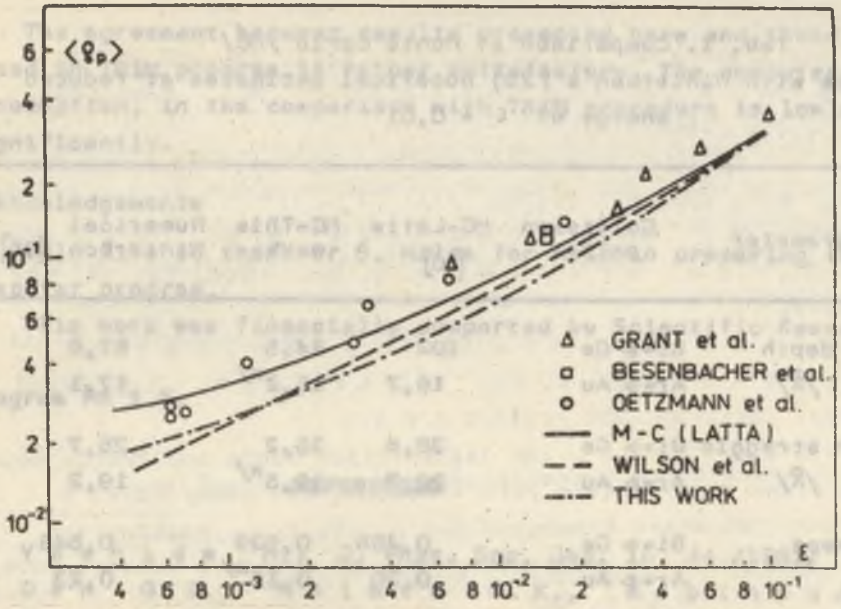

Fig. 7. Reduced mean projected range ϱ_p versus reduced energy ε, /Experimental and theoretical data compilation of Latta [10]/Experimental data: O - Oetzmann et al. [21], Δ - Grant et al. [22], □ - Besenbacher et al. [23].

We also compare the values of the higher moments /skewnes and kurtosis/ with those calculated by Latta [10]. The results are summarised in Tab. 1.

The results of the calculations presented above indicate rather good agreement with other theoretical results and also with experimental measurements except the heavy ions implantation /see Fig. 5 and 7/. In this case the theoretical predictions are lower than those of the experiment. All theoretical curves /Fig. 7/ converge at the largest ε value. At low ε values the best fit to the experimental data are obtained when Monte-Carlo treatment for Solid State Thomas-Fermi /SSTF/ potential /Latta [10] / is used. In general, neither Thomas-Fermi potential nor SSTF and Molier approximation to the Thomas-Fermi screening function, results in mean-depth estimates that would agree with experiment over the full ε range [10, 11].

Tab. 1. Comparison of Monte Carlo /MC/ results with Winterbon's [25] numerical estimates at reduced energy of $\varepsilon = 0{,}01$

Parameter	Collision pair	MC-Latta [10]	MC-This work	Numerical Winterbon [25]
Mean depth	Bi⇒Ge	102	84,5	67,6
$\langle x \rangle$ /Å/	Ar⇒Au	18,7	16,2*/	17,1
Depth straggle	Bi⇒Ge	38,5	35,2	25,7
σ /Å/	Ar⇒Au	22,7	19,5*/	19,2
Skewness	Bi⇒Ge	0,485	0,539	0,546
S	Ar⇒Au	0,20	0,15*/	0,23
Kurtosis	Bi⇒Ge	3,32	3,43	3,23
K	Ar⇒Au	3,21	3,45*/	3,18

*/ - calculated for infinite medium

4. CONCLUSION

In the paper we have presented the simple Monte Carlo simulation procedure of slowing down of energetic ions in amorphous materials. One of the features of this program which distinguishes it from other procedures is the use of extremely simplified analytic expression of scattering angle and energy loss evaluation. The other one is connected with electronic stopping cross section treatment, in which we propose an alternative approximation to the impact parameter dependence of the electronic energy loss.

To save computer time usage in the case of high energies calculations the simple impact parameter selection procedure is presented.

The agreement between results presented here and those based on TRIM program is rather satisfactory. The computer time consumption, in the comparison with TRIM procedure is lowering significantly.

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STRESZCZENIE

W pracy przedstawiono uproszczoną metodę Monte-Carlo określenia parametrów głębokościowych rozkładów jonów implantowanych do tarcz amorficznych. W obliczeniach przeprowadzonych dla kilku kombinacji jon-tarcza wykorzystano potencjał Moliera. Otrzymane wyniki porównano z obliczeniami teoretycznymi i wynikami doświadczalnymi innych autorów.

Р Е З Ю М Е

В работе представлен модифицированный метод Монте-Карло определения концентрационных распределений имплантированных ионов в аморфные мишени. Расчеты проводились для нескольких пар ион-мишень с потенциалом Мольера. Полученные результаты сравниваются с теоретическими предсказаниями и экспериментальными данными других авторов.

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