DISTRIBUTIONS OF ENERGY LOSSES BY FAST IONS ALONG THEIR PROPAGATION PATHS IN SOLIDS

V.V. ILYINA, M.V. MAKARETS

Taras Shevchenko National University of Kyiv
(64, Volodymyrs'ka Str.,01033 Kyiv, Ukraine; e-mail: mmv@univ.kiev.ua)

PACS 61.72.uf; 61.72.uj; 61.80.-x

The integro-differential equations for cumulants of the distribution function that describes energy losses by fast ions during their propagation in solids have been obtained. The equations differ from those obtained by other authors by one new term. The term describes accurately the process of slowing down of an ion at the start of its path. The equations have been numerically solved for the first seven cumulants of the distribution function for both elastic and inelastic energy losses, and the results have been compared with the results for ion ranges. It has been found that: 1) for energies in the interval 1 keV-1 GeV, the average ranges with energy losses are approximately 30-90% of the ion ranges; 2) for low energies, the straggling of the distribution of energy losses are slightly larger than or equal to the straggling of the distribution of ion ranges, while, for high energies, the former can be 10 times as large as the latter; 3) for low energies, the skewnesses and excesses of the distributions of energy losses and ion ranges are approximately the same, while their changes for the former at higher energies are several orders smaller than those for the latter. This implies that the distribution of energy losses are wider and closer to the normal distribution than the distribution of ion ranges. We show that these properties of energy loss distributions are a result of the inclusion of the new terms in the equations which dominate at high energies.

1. Introduction

The first system of equations for the distribution function of ions implanted into a solid was obtained over half a century ago [1]. The methods to study these equations have been developed in several stages [2,3]. In the recent years, the authors of [4–6] have proposed the *cumulant approach* and developed numerical methods that allow cumulants up to the 6th order to be calculated and analyzed for the whole energy range, where the assumptions of the classical implantation theory [1] hold.

The main advantage of this approach is that cumulants of the distribution are smoother functions of the ion energy than its moments – their amplitudes are less by several orders. It has allowed one to find an exact enough analytical approximation and construct a stable numerical method. In general, the hardly soluble equations with the obvious physical meaning were reduced to a more easily soluble equation but with a more fuzzy physical meaning.

Now we use the cumulant approach for the investigation of energy losses of fast ions in a solid.

When we have applied this approach for the first time to equations from [7] which describe the energy loss distributions of ions and knocked-out particles, we obtained unexpected results. Namely, the norm and other cumulants of the nuclear energy losses distribution were equal to zero. On the contrary, the norm of the electronic energy losses distribution was equal to the ion energy E, and its other cumulants were also non-zero. These results contradict the physical meaning, but the sum of norms is in complete agreement with the energy conservation law.

We felt obliged to investigate the reasons for having the solution to the well-established equations that contradicts the basic physics laws. This investigation [8] has shown that the equations for the spatial energy losses [2, 7] contain a hidden assumption that the Energy Loss Distribution (ELD) function for an ion at the start of its path has a zero value. This assumption is a consequence of the even earlier assumption that the losses inside an infinitely small volume δV are proportional to δV.

The same assumption was made while obtaining the equations for the ranges of implanted ions [1]. In this case, however, the assumption is completely valid, because an ion cannot stop more than once inside δV. Therefore, the number of random stops is $\delta n = 1$ if an ion stopped inside δV and $\delta n = 0$ if an ion stopped outside δV. Then, using the first-order approximation, it can be assumed that an ion takes up a volume of $\Delta V \approx 1/N_0$, where N_0 is the atom concentration of a solid. Then the probability of the ion stopping in a volume $\delta V \leq \Delta V$ is defined as $\delta\mathcal{P} \approx \delta n \delta V/\Delta V \sim \delta V$ and has a norm equal to 1. Then we can introduce a density of implanted ions as a limit $\Pi(\vec{r}, E) = \lim\limits_{\delta V \to 0} \delta\mathcal{P}/\delta V$. In the same way, one can introduce the density of the ions distribution along their paths by considering an infinitely small length δl.

Let us now consider the energy losses of an ion. While an ion only stops once, it looses energy in many collisions during its trajectory. Energy losses can occur many times in the same volume δV if the characteristic length of a collision-free path of an ion λ is small or if ion's trajectory is very complex. Therefore, an ion passes through the same volume δV many times before leaving it or stopping in it, and thus the energy lost in δV will be equal to 0 if an ion did not cross δV or proportional to a number of collisions δn if an ion crossed δV.

Now, the number of random collisions inside δV is $\delta n \approx \delta l/\lambda$, where $\delta l \sim (\delta V)^{1/3}$ is the ion path, and we can assume in the first-order approximation that the energy is transferred from an ion to a solid through a cylinder with a volume $\Delta V \approx \pi R^2 \lambda$. The axis of the cylinder connects the locations of two neighboring collisions. For elastic collisions, the radius of the cylinder R_n is equal to the half-distance between atoms of a solid $R_n \approx a/2$. For inelastic collisions, the radius R_e depends on the ion energy and the properties of the electronic subsystem of a solid [9]. It can be defined generally as $R_e \equiv R(E, N_0, \ldots)$.

If we denote the energy lost in one collision of the α-type (where $\alpha = n, e$ for nuclear and electronic collisions) as $\langle T^\alpha \rangle$, then the probable loss of energy inside $\delta V \leq \Delta V$ can be determined from $\delta \mathcal{P}^\alpha \approx \langle T^\alpha \rangle \delta n \delta V / \Delta V$. This probability has a norm of $\kappa_0^\alpha(E)$, which is the energy lost in one collision of the α-type. It follows from here that $\delta \mathcal{P}^\alpha \sim (\delta V)^{4/3}$, and therefore we cannot determine the volume density for energy losses, at least within the limits of this approach. However, we can introduce the density of energy losses along an ion's path δl if we consider the probable loss of energy $\delta \mathcal{P}^\alpha \approx \langle T^\alpha \rangle \delta n \sim \delta l$.

2. Main Equations and Their Analysis

In this paper, we consider the distribution functions for energy losses per unit length of an ion along its trajectory in the solid. To be more precise, we study the cumulants of these distributions.

Let $\Pi^\alpha(E, R)dR$ be the most probable energy lost by a fast ion with initial energy E in the α-type collision in the vicinity of a point dR along ion's path R, where $\alpha = t, n, e$ correspond to the total, nuclear, and electronic losses, respectively. We follow [1] to obtain the equations for the density of the distribution:

$$\frac{\partial \Pi^\alpha(E,R)}{\partial R} = -N_0 \int d\sigma(E,T) \left\{ \Pi^\alpha(E,R) - \right.$$
$$\left. - \Pi^\alpha(E-T,R) \right\}, \qquad (1)$$

where $d\sigma(E,T)$ is the differential cross-section of the elastic and inelastic scattering process involving the ion and a target atom, and T is the energy lost in this scattering process.

This equation is identical in form to the equation for the density distribution of ion ranges obtained in [1]. However, the meaning of the function $\Pi^\alpha(E,R)$ is different from the one used in [7]. This leads to an initial condition (at $R = 0$) for this function being different from the one used in [2, 7].

Namely, the function $\Pi^e(E,0)dR$ for electronic losses is the most probable energy lost in inelastic collisions during the path dR near the start point of an ion. Then it follows that $\Pi^e(E,0) = S_e(E)$, where $S_e(E) \equiv \int T_e d\sigma_e(E,T_e)$ is the inelastic energy loss per unit length of an ion with energy E or the electronic stopping, and $d\sigma_e(E,T_e)$ is the differential cross-section of electronic scattering.

For nuclear losses, $\Pi^n(E,0) = S_n(E)$, where $S_n(E) \equiv \int T_n d\sigma_n(E,T_e)$ is the elastic energy loss per unit length of an ion with energy E or the nuclear stopping, and $d\sigma_n(E,T_n)$ is the differential cross-section of nuclear scattering. It is obvious that, for the total losses, $\Pi^t(E,0) = S_e(E) + S_n(E)$.

Therefore, for the α-type losses, we can write down $\Pi^\alpha(E,0) = S_\alpha(E)$, where $S_\alpha(E)$ is the α-type stopping for an ion with energy E. These initial conditions mean that a fast ion will start to loose energy immediately after the start.

We can also include the ion ranges distribution in the common scheme of energy losses calculations, if we taken its initial condition $\Pi(E,0) = 0$ into account and then set the index $\alpha = i$ and formally put $S_i(E) = 0$. In this case, the most probable number of ions which are stopped at the start is zero, but there is no reason to believe that this initial condition holds for energy losses. Since this zero initial condition was incorrectly used in [2, 7] for the elastic energy loss distribution of fast particles stopped into a unit volume, the corresponding equations have the above solutions.

Let us now change to the Lindhard's dimensionless units by replacing $R \Rightarrow \rho$ and $E \Rightarrow \varepsilon$ following [1, 2] in Eq. (1). We will also replace the function $\Pi^\alpha(\varepsilon, \rho)$ by its cumulants κ_k^α, where $k = 0, 1, 2, \ldots$, following [4]. Taking the norm of the energy distribution function as the energy lost in an α-type collision $\kappa_0^\alpha(\varepsilon)$, we can write down the following expression for the energy loss distribution density func-

tion [4]:

$$\Pi^{\alpha}(\varepsilon,\rho)=\frac{\kappa_0^{\alpha}}{\pi\,\Delta\rho^{\alpha}}\int_0^{\infty}\exp\left[-\frac{1}{2!}s^2+\frac{Ex_1^{\alpha}}{4!}s^4-\frac{Ex_2^{\alpha}}{6!}s^6+\ldots\right]\times$$

$$\times\cos\left[-r^{\alpha}s-\frac{Sk_1^{\alpha}}{3!}s^3+\frac{Sk_2^{\alpha}}{5!}s^5-\ldots\right]ds, \tag{2}$$

where $\Delta\rho^{\alpha}=\sqrt{\kappa_2^{\alpha}(\varepsilon)/\kappa_0^{\alpha}(\varepsilon)}$ is the straggling of the mean path $\rho^{\alpha}(\varepsilon)=\kappa_1^{\alpha}(\varepsilon)/\kappa_0^{\alpha}(\varepsilon)$, $r^{\alpha}\equiv r^{\alpha}(\rho,\varepsilon)$ is the centered dimensionless mean ion path, and Sk_j^{α} and Ex_j^{α} are the distribution's skewness and excess, respectively, which depend on the energy ε only. These quantities can be expressed through the cumulants by

$$r^{\alpha}=\frac{\rho-\rho^{\alpha}(\varepsilon)}{\Delta\rho^{\alpha}(\varepsilon)},\quad Sk_j^{\alpha}=\frac{\kappa_{2j+1}^{\alpha}(\varepsilon)}{\kappa_0^{\alpha}(\varepsilon)\left[\Delta\rho^{\alpha}(\varepsilon)\right]^{2j+1}},$$

$$Ex_j^{\alpha}=\frac{\kappa_{2j+2}^{\alpha}(\varepsilon)}{\kappa_0^{\alpha}(\varepsilon)\left[\Delta\rho^{\alpha}(\varepsilon)\right]^{2j+2}},\quad j=1,2,\ldots \tag{3}$$

At a fixed ion energy ε, $r^{\alpha}(\rho)$ is the dimensionless distribution's variable, and Sk_j^{α} and Ex_j^{α} are dimensionless distribution's parameters. The cumulant of the jth order has the units of $(\text{length})^j$ multiplied by the units of κ_0^{α}. It follows from Eq. (2) that the cumulant κ_0^{α} defines the amplitude of the distribution, while its form depends on the parameters $\chi_j^{\alpha}(\varepsilon)=\kappa_j^{\alpha}(\varepsilon)/\kappa_0^{\alpha}(\varepsilon)$, where $j=1,2,\ldots$ Equations (2) and (3) remain true for the ion ranges distribution, since $\kappa_0^{i}(\varepsilon)\equiv 1$.

Following [4] and using Eq. (1), we obtain the equations for the cumulants using the initial condition $\Pi^{\alpha}(E,0)=S_{\alpha}(\varepsilon)$. For the norm of the distribution function κ_0^{α} and the mean path distribution κ_1^{α}, these equations become

$$\hat{\mathcal{L}}\left\{\kappa_0^{\alpha}\right\}=S_{\alpha}(\varepsilon), \tag{4}$$

$$\hat{\mathcal{L}}\left\{\kappa_1^{\alpha}\right\}=\kappa_0^{\alpha}(\varepsilon), \tag{5}$$

where the left-hand operator is defined as

$$\hat{\mathcal{L}}\left\{\kappa_k^{\alpha}\right\}\equiv\hat{\mathcal{N}}\left\{\kappa_k^{\alpha}(\varepsilon-\gamma\tau)\right\}+S_e(\varepsilon)\frac{\partial\kappa_k^{\alpha}(\varepsilon)}{\partial\varepsilon}, \tag{6}$$

$$\hat{\mathcal{N}}\left\{\ldots\right\}\equiv-\frac{1}{\gamma}\int_0^{\varepsilon}\sigma(\varepsilon,\tau)\frac{\partial}{\partial\tau}\left\{\ldots\right\}d\tau, \tag{7}$$

where $\hat{\mathcal{N}}$ is the nuclear scattering operator, $\sigma(\varepsilon,\tau)$ is defined in [4] as the so-called summarized cross-section of ion's nuclear scattering on the target atom, $\gamma=4M_1M_2/\left(M_1+M_2\right)^2$, and $M_{1,2}$ are the masses of an ion and the target atom, respectively.

The equations for the cumulants of the $k\geq 2$ order are:

$$\hat{\mathcal{L}}\left\{\kappa_k^{\alpha}\right\}=\hat{\mathcal{N}}\left\{\kappa_0^{\alpha}(\varepsilon-\gamma\tau)F_k\left(\chi_1^{\alpha},\ldots,\chi_{k-1}^{\alpha}\right)\right\}+$$
$$+S_{\alpha}(\varepsilon)f_k\left(\chi_1^{\alpha},\ldots,\chi_{k-1}^{\alpha}\right), \tag{8}$$

where the functions $F_k(\chi_1^{\alpha},\ldots,\chi_{k-1}^{\alpha})$ and $f_k(\chi_1^{\alpha},\ldots,\kappa_{k-1}^{\alpha})$ do not depend on the type of a collision explicitly. In particular, for the cumulants of the second-sixth orders which define the straggling, two skewnesses, and two excesses, the functions F_k do not depend on the norm κ_0^{α} explicitly:

$$F_2=\left[\Delta_1^{\alpha}(\varepsilon,\tau)\right]^2, \tag{9}$$

$$F_3=\Delta_1^{\alpha}(\varepsilon,\tau)\left\{\left[\Delta_1^{\alpha}(\varepsilon,\tau)\right]^2+3\Delta_2^{\alpha}(\varepsilon,\tau)\right\}, \tag{10}$$

$$F_4=\Delta_1^{\alpha}(\varepsilon,\tau)\left\{\left[\Delta_1^{\alpha}(\varepsilon,\tau)\right]^3+6\Delta_2^{\alpha}(\varepsilon,\tau)\Delta_1^{\alpha}(\varepsilon,\tau)+\right.$$
$$\left.+4\Delta_3^{\alpha}(\varepsilon,\tau)\right\}+3\left[\Delta_2^{\alpha}(\varepsilon,\tau)\right]^2, \tag{11}$$

$$F_5=\Delta_1^{\alpha}(\varepsilon,\tau)\left\{\left[\Delta_1^{\alpha}(\varepsilon,\tau)\right]^4+10\Delta_2^{\alpha}(\varepsilon,\tau)\left[\Delta_1^{\alpha}(\varepsilon,\tau)\right]^2+\right.$$
$$+10\Delta_3^{\alpha}(\varepsilon,\tau)\Delta_1^{\alpha}(\varepsilon,\tau)+15\left[\Delta_2^{\alpha}(\varepsilon,\tau)\right]^2+$$
$$\left.+5\Delta_4^{\alpha}(\varepsilon,\tau)\right\}+10\Delta_2^{\alpha}(\varepsilon,\tau)\Delta_3^{\alpha}(\varepsilon,\tau), \tag{12}$$

$$F_6=\Delta_1^{\alpha}(\varepsilon,\tau)\left\{\left[\Delta_1^{\alpha}(\varepsilon,\tau)\right]^5+15\Delta_2^{\alpha}(\varepsilon,\tau)\left[\Delta_1^{\alpha}(\varepsilon,\tau)\right]^3+\right.$$
$$+20\Delta_3^{\alpha}(\varepsilon,\tau)\left[\Delta_1^{\alpha}(\varepsilon,\tau)\right]^2+15\Delta_4^{\alpha}(\varepsilon,\tau)\times$$
$$\times\Delta_1^{\alpha}(\varepsilon,\tau)+45\left[\Delta_2^{\alpha}(\varepsilon,\tau)\right]^2\Delta_1^{\alpha}(\varepsilon,\tau)+$$
$$\left.+60\Delta_2^{\alpha}(\varepsilon,\tau)\Delta_3^{\alpha}(\varepsilon,\tau)+6\Delta_5^{\alpha}(\varepsilon,\tau)\right\}+$$
$$+15\left[\Delta_2^{\alpha}(\varepsilon,\tau)\right]^3+10\left[\Delta_3^{\alpha}(\varepsilon,\tau)\right]^2+$$
$$+15\Delta_2^{\alpha}(\varepsilon,\tau)\Delta_4^{\alpha}(\varepsilon,\tau), \tag{13}$$

where $\Delta_i^{\alpha}(\varepsilon,\tau)=\chi_i^{\alpha}(\varepsilon-\gamma\tau)-\chi_i^{\alpha}(\varepsilon)$, and $\Delta_i^{\alpha}(\varepsilon,0)=0$ for all i. The functions f_k are obtained from F_k by the substitution $\chi_j^{\alpha}(\varepsilon-\gamma\tau)=0$ for $j=1,2,\ldots,k-1$.

Note that the equations for the cumulants contain the terms which are proportional to $S_{\alpha}(\varepsilon)$ on the right-hand side and take the energy losses of an ion at the start of its path into account.

Equations (4), (5), and (8) are inhomogeneous second-order Volterra-type integral equations with integrable singularity core $\sigma(\varepsilon,\tau\to 0)\to\infty$ [4] which describe the first derivative of the cumulants. They have non-trivial solutions only if the right-hand sides are non-zeros [10]. The equations should be solved one by one, since Eq. (4) has the explicitly given right-hand side.

The ion ranges distribution is an example where the contribution of $S_{\alpha}(\varepsilon)$ is equal to zero. In this case, Eq.

(4) for the norm becomes homogeneous with respect to its derivative,

$$\int_0^{\varepsilon} \sigma(\varepsilon,\tau)\left\{\frac{\partial\kappa_0^i(\varepsilon-\gamma\tau)}{\partial\varepsilon}\right\}d\tau + S_e(\varepsilon)\frac{\partial\kappa_0^i(\varepsilon)}{\partial\varepsilon} = 0, \quad (14)$$

and has the trivial solution $\frac{\partial\kappa_0^i(\varepsilon)}{\partial\varepsilon} = 0$. Using the norm conditioning it follows that $\kappa_0^i(\varepsilon) \equiv 1$, and Eq. (5) reduces to the equations for ranges obtained in [1]. For the cumulants of order $k \geq 2$, the right-hand sides of Eqs. (8) do not contain the second term, and the integrals in Eqs. (9)–(11) coincide with the results obtained in [4].

Therefore, we have shown that while the equations for the ion ranges distribution functions and the ELD functions are the same, the equations for their cumulants, moments, and central moments differ. The reason for this is that while it is very unlikely that an ion will stop right at the beginning of its path, it is almost certain that it will loose some energy at the beginning of its path. The consequence of this difference is the different initial conditions for the distribution functions which define the right-hand sides of the equations for the cumulants of these distributions.

3. Results and Discussion

The first-order series expansions of the integral functions, Eqs. (4) and (5), for the energy loss $\gamma\tau$ allows us to obtain the analytical approximations for the norm of the distribution function and for the mean path:

$$\kappa_0^{\alpha}(\varepsilon) \approx \int_0^{\varepsilon} \frac{S_{\alpha}(\varepsilon')}{S_n(\varepsilon')+S_e(\varepsilon')}d\varepsilon', \quad (15)$$

$$\rho^{\alpha}(\varepsilon) \approx \frac{1}{\kappa_0^{\alpha}(\varepsilon)}\int_0^{\varepsilon} \frac{\kappa_0^{\alpha}(\varepsilon')}{S_n(\varepsilon')+S_e(\varepsilon')}d\varepsilon'. \quad (16)$$

Approximation (15) satisfies the energy conservation law, because $\kappa_0^t(\varepsilon) = \varepsilon$, and the integrands in this equation can be interpreted as the probability of the energy losses of the α-type per unit path of an ion with the energy ε'. To our knowledge, the equations have not been presented elsewhere. Expression (16) is a generalization of a well-known result for the ion mean range [1].

We have solved Eqs. (4), (5), and (8) numerically, by using the method developed in [4, 5]. Within this method, the left-hand sides of the equations are transformed into a system of linear equations for the expansion coefficients $\kappa_i^{\alpha}(\varepsilon)$. The expansion is carried out for the energy intervals, whose lengths grow geometrically until they cover the range of energies, where the assumptions of binary elastic ion-atom collisions hold.

For the lower energy limit, we assume the energy, for which the distance between an ion and an atom during the head-on collision is 1/4 of the half-distance of atoms in the target. For the upper energy limit, we assume the energy, for which the distance between an ion and an atom during the head-on collision is 1/4 of the sum of their radii and the radius of the nuclear force action. For inelastic and elastic collisions, we use, respectively, the approximation of [11] and the potential proposed by Ziegler–Biersack–Littmark [12].

In Fig. 1, we show the dependences $\kappa_0^{t,n,e}(\varepsilon)$ and $\kappa_0^{t,n,e}(\varepsilon)/\varepsilon$ calculated for the implantation of phosphorus ions into a silicon target. The lower and upper energy limits are chosen to represent energies, where the assumptions of [1] hold. They are equal to 2.8 keV and 281 MeV, respectively. We have chosen this ion-target combination because of its practical applications, but also because $\gamma \approx 1$ for this combination, and the expansion in γ in integrands has the worst asymptotic behavior.

One can see from Fig. 1,*a* that, for large energies, nearly all losses are caused by the electronic scattering, however the nuclear losses slowly increase as well. We can see from Fig. 1,*b* that the energy lost in elastic, inelastic, and all collisions satisfies the energy conservation law, though it has not been used in obtaining the equations. We believe that the accuracy, to which the law is satisfied (more than 0.2%), can be interpreted as the indirect evaluation of the numerical method accuracy.

To approximate the equations for cumulants of the order $k \geq 2$ analytically, we have to take into account the expansion of the integrands F_k in Eq. (8) in $\gamma\tau$ up to the second-order terms. Therefore, the approximation of the integral begins with the straggling of the nuclear scattering $W(\varepsilon) = \int \tau^2 d\sigma(\varepsilon,\tau) = 2\int \tau\sigma(\varepsilon,\tau)d\tau$. The right-hand sides have the term proportional to $S_{\alpha}(\varepsilon)$, and we can rewrite the equations as

$$\{S_n(\varepsilon)+S_e(\varepsilon)\}\frac{\partial\kappa_k^{\alpha}(\varepsilon)}{\partial\varepsilon} \approx S_{\alpha}(\varepsilon)f_k\left(\chi_1^{\alpha},\ldots,\chi_{k-1}^{\alpha}\right) + \\ + \frac{1}{2}W(\varepsilon)\kappa_0^{\alpha}(\varepsilon)F_k^{(2)}\left(\chi_1^{\alpha},\ldots,\chi_{k-1}^{\alpha}\right), \quad (17)$$

where $F_k^{(2)}$ is the second derivative of F_k with respect to τ at $\tau = 0$, which is a polynomial of the second order in the first derivatives of the cumulants of the $(k-1)$th order inclusive. In case of the distribution

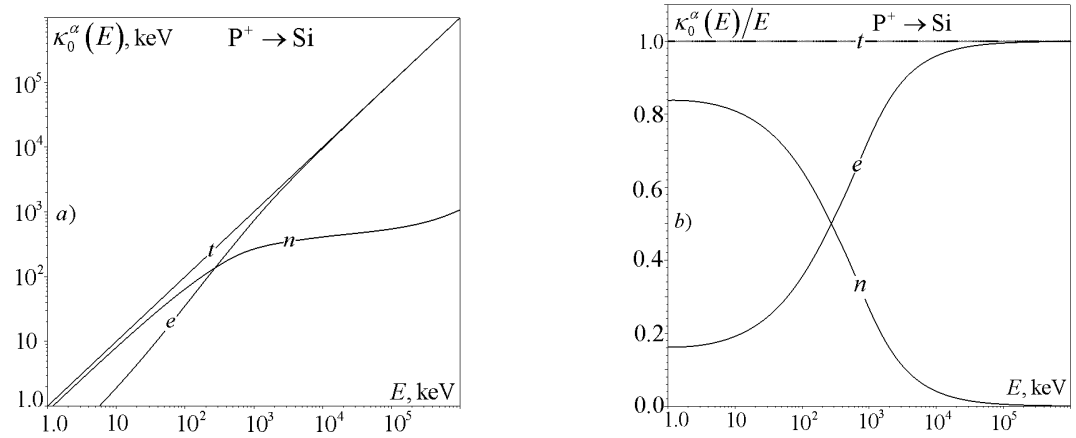

Fig. 1. Dependence of the norm of the energy losses function – *a* and the relative norm – *b* on the implantation energy of phosphorus ions into a silicon target. Letters n, e, and t next to the curves denote the distributions of nuclear, electronic, and total losses, respectively

of ranges, when $\kappa_0^\alpha(\varepsilon) \equiv 1$ and $S_i(\varepsilon) \equiv 0$, the right-hand sides of Eq. (17) can be simplified, and the first derivative of the cumulant of the kth order can be expressed through the moments of nuclear scattering explicitly [4]. In the case of energy losses, the second term on the right-hand side of Eq. (17) is proportional to the cumulants of the $(k-1)$th order, and this can change the dependence of cumulants on energy significantly.

Figure 2 presents the graphs of dependences of parameters from Eqs. (2) and (3) on the ion energy for the distributions $\alpha = n,\ e,\ t$ and i for the combination phosphorus-silicon. The arrow and the number in Fig. 2,*c–f* near the curve for the parameter of the ions distribution show the direction of its monotonic change and its value for an ion energy of 1 GeV, respectively.

One can see from Fig. 2,*a* that the mean of the total ELD is smaller than the mean of the ions distribution corresponding to the picture of the energy losses of an ion just before it stops. One can also see that the mean of the elastic losses distribution and the ranges distribution have similar values for high energies suggesting that this mechanism dominates at the end of the ion path, when its energy is low. Stragglings of losses of all types, Fig. 2,*b*, exceed the straggling of the ranges distribution, by suggesting that the energy losses are distributed more evenly during the ion path. Therefore, the ELDs will have maxima toward the beginning of its path, and the distributions will be wider than the ranges distribution. In addition, the ratio of the straggling to the mean $\Delta\rho^\alpha/\rho^\alpha$ has a maximum for the total losses distribution and has a minimum for the ranges distribution. Therefore, these distributions will be narrower and wider, respectively.

Figure 2,*c–f* demonstrates the common property for all parameters of the order $k \geq 3$ for the ELDs, which is their relatively small change of amplitudes. Namely, the changes in amplitudes for the ELDs are several times smaller than those for the ranges distribution. Then it follows that these distributions are closer to the normal distribution, as all cumulants of the order $k \geq 3$ are equal to zero [13]. We can also see that the parameters for the total loss distribution for low energies are similar to parameters for the elastic loss distribution, while, for high energies, they become similar to the parameters for the inelastic energies distribution. This corresponds to the fact that different loss mechanisms dominate at different energies.

We can now conclude that, for the ELDs for different types of collisions, we can use the normal distribution as the zero-order approximation. An indirect criterion for its applicability will be the initial condition $\Pi^\beta(E,0) = S_\beta(E)$ for $\beta = n, e, t$ which can be written explicitly as

$$\frac{\kappa_0^\beta(\varepsilon)}{\sqrt{2\pi}\,\Delta\rho^\beta(\varepsilon)} \exp\left\{-\frac{1}{2}\left[\frac{\rho^\beta(\varepsilon)}{\Delta\rho^\beta(\varepsilon)}\right]^2\right\} \approx S_\beta(E). \qquad (18)$$

This condition links three first cumulants. We have also calculated the ratio of the left-hand side of Eq. (18) to its right-hand side for the phosphorus/silicon combination. The value of this ratio shows that the normal distribution at $|Sk|, |Ex| \leq 1$ gives values of the ELDs at the coordinate origin that are approximately 1/3 of the true values. If $|Sk|$ and $|Ex|$ are large, then the difference increases further, and it becomes necessary to use one of

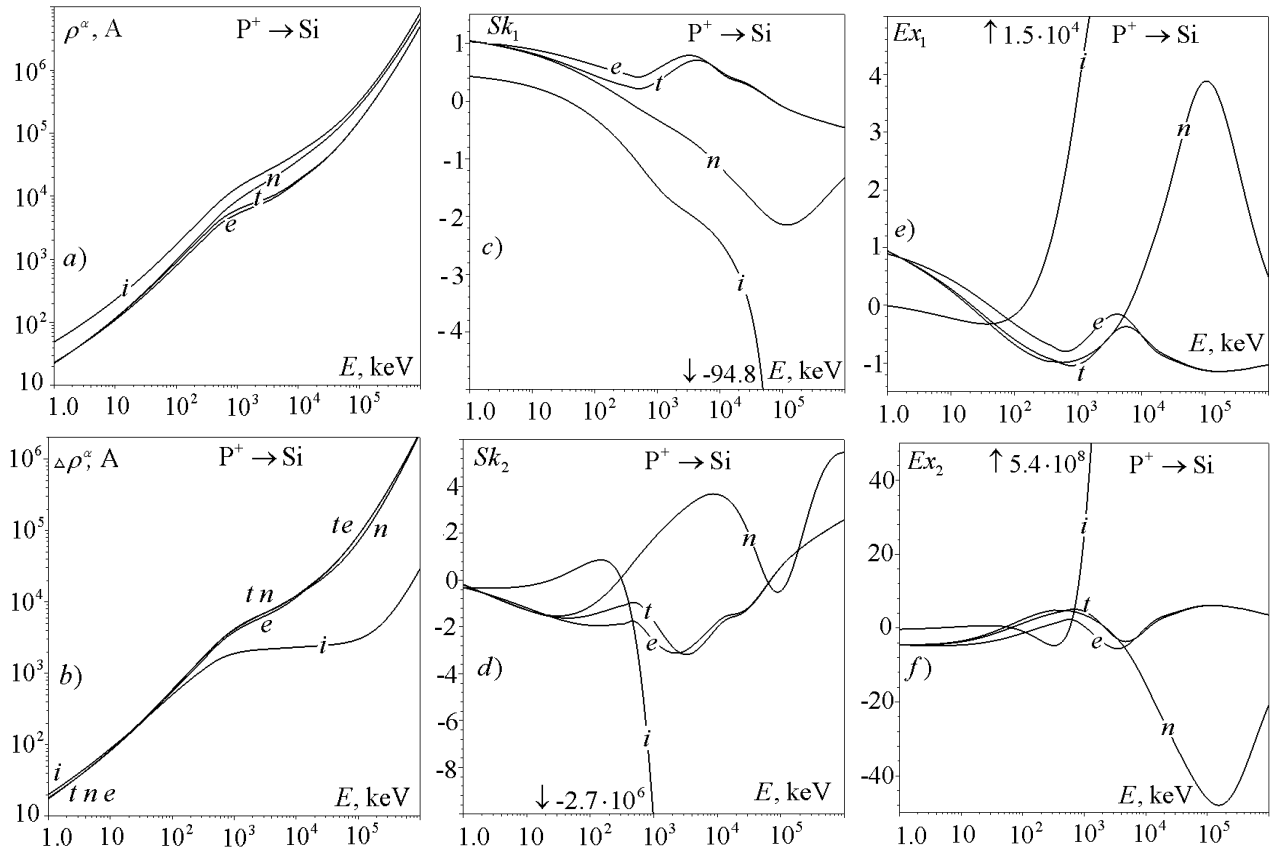

Fig. 2. Dependence on the implantation energy of phosphorus ions into a silicon target for: *a, b* – mean path distribution and its straggling; *c, d* – the first and second skewnesses; *e, f)* – the first and second excesses. The letter *i* near the curves denotes the ion distribution

the Pearson distributions [2] or the Johnson distribution [14].

We have also carried out the numerical analysis of the contributions of both members on the right-hand side of Eq. (8). The analysis has shown that the stopping member with $S_\alpha(\varepsilon)$ dominates, while the nuclear scattering only contributes significantly at low energies. This justifies the use of the approximation

$$\chi_k^\alpha(\varepsilon) \approx \frac{1}{\kappa_0^\alpha(\varepsilon)} \int_0^\varepsilon \frac{S_\alpha(\varepsilon') f_k\left(\chi_1^\alpha(\varepsilon'), \ldots, \chi_{k-1}^\alpha(\varepsilon')\right)}{S_n(\varepsilon') + S_e(\varepsilon')} d\varepsilon', \tag{19}$$

for $k \geq 2$. The analysis has shown that, for all ion-target combinations, the error of approximations (15), (16), and (17) is the largest for $k = 2$, when $M_1 \approx M_2$. For all types of losses, the error of the norm can be negative or positive and generally does not exceed 5%. For the mean and the straggling, the results of using this approximation gives values which are smaller than true ones by no more than 15% and 25%, respectively. The skewnesses and excesses change the sign, and the errors can be large.

In Fig. 3, we show the comparison of the numerical results obtained by solving Eqs. (4), (5), and (8) and the results obtained using approximations for the implantation of boron ions in a germanium target.

One can see from Fig. 3 that the approximate values of the parameters of the order $k \geq 3$ are very close to the calculated values for high energies. For low energies, the approximate values have the correct order of magnitude and the general dependence structure. The maximum errors for the mean and the straggling occur for the same energies. Therefore, we can use the approximations in Eqs. (15), (16), and (17) or (19) for estimating the cumulants for the whole energy range used in the implantation.

The results above show that, for the ELDs of various types, we can use the Gaussian distribution for the zero-order approximation. This approximation will be

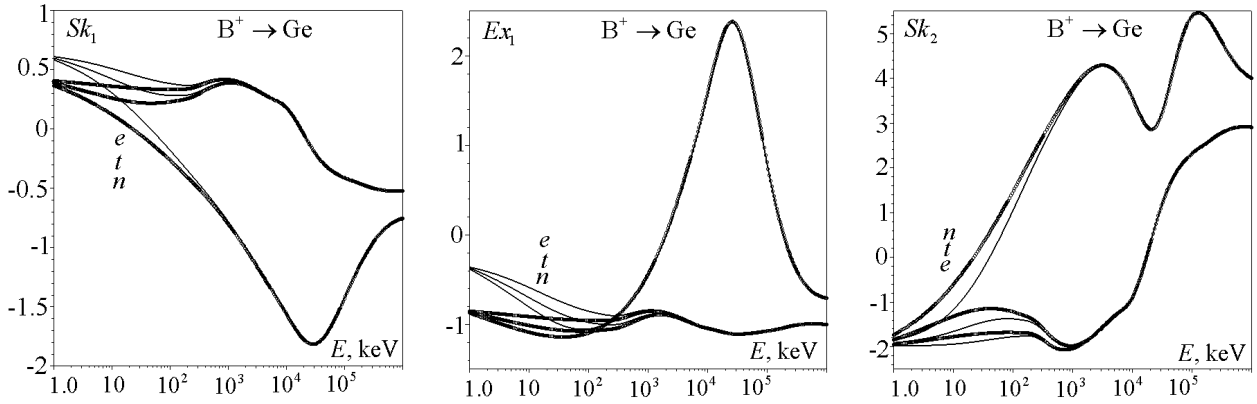

Fig. 3. Parameters for the ELDs for the implantation of boron ions into the germanium target. Solid lines denote the numerical solutions, and the dotted lines denote the approximations

true for the whole energy range used in the implantation. If the parameters of higher order are large enough to distort the Gaussian distribution [2], we can use the Pearson-4 distribution.

4. Conclusions

In the present work, it is shown that it is necessary to take into account in equations for the cumulants of the energy loss distribution (ELD) function that the energy loss is a continuous process, while the stop of an ion is an event. Therefore, the energy losses happen continuously along the whole path of an ion with high probability, while the probability of the ion stopping at the beginning of its path is very low.

Accounting for these differences leads to different initial conditions that must be used in the equations for the range distributions and ELDs. As a consequence, the equations for the cumulants of the loss distribution functions have additional terms on the right-hand side which are proportional to the stopping per unit length. This term gives the main contribution into the values of the cumulants and the corresponding parameters. On the other hand, the equations for the cumulants of the range distribution function do not contain this term and account only for nuclear scattering, which makes a contribution to the values of the cumulants of the ELD function to be insignificant.

1. J. Lindhard, M. Scharf, and H.E. Schiott, Kgl. Danske Videnskab. Selskab, Mat.-Fys. Medd. **33**, No. 14, 1 (1963).

2. A.F. Burenkov, F.F. Komarov, M.A. Kumakhov, and M.M. Temkin, *Tables of Parameters of the Spatial Distribution of an Implanted Admixture* (Bel. State Univ., Minsk, 1980) (in Russian).

3. D.G. Ashworth, M.D.J. Bowyer, and R.J. Oven, J. Phys. D: Appl. Phys. A **24**, 1376 (1991).

4. M.V. Makarets and S.N. Storchaka, Ukr. Fiz. Zh. **46**, 486 (2001).

5. V.V. Ilyina and M.V. Makarets, Ukr. Fiz. Zh. **49**, 815 (2004).

6. M.V. Makarets, V.V. Ilyina, and V.V. Moskalenko, Vacuum. **78**, 381 (2005).

7. J. Lindhard, V. Nielsen, M. Scharff, and P.V. Thomsen, Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd. **33**, No. 10, 1 (1963).

8. V.V. Ilyina and M.V. Makarets, *Abstr. of the 2nd Conference FMMN'2008* (SCPT, Kharkiv, 2008), **2**, p. 534.

9. E.G. Gamaly and L.T. Chaddernon, Proc. Roy. Soc. Lond. **449**, 381 (1995).

10. A.D. Polyanin and A.V. Manzhirov, *Handbook of Integral Equations* (CRC Press, Boca Raton, 1998).

11. www.srim.org

12. J.F. Ziegler, J.P. Biersack, and U. Littmark, *The Stopping and Ranges of Ions in Solids* (Pergamon Press, New York, 1985), V.1.

13. W. Feller, *An Introduction to Probability Theory and Its Applications* (Wiley, New York, 1970).

14. M.D.J. Bowyer, D.G. Ashworth, and R. Oven, J. Phys. D: Appl. Phys. **29**, 1274 (1996).

Received 07.07.09

РОЗПОДІЛ ВТРАТ ЕНЕРГІЇ ШВИДКИХ ІОНІВ ВЗДОВЖ ЇХ ШЛЯХУ У ТВЕРДОМУ ТІЛІ

В.В. Ільїна, М.В. Макарець

Р е з ю м е

Отримано інтегродиференціальні рівняння для кумулянтів функції розподілу втрат енергії швидких іонів вздовж їх шляху у твердому тілі, у яких враховано втрати енергії починаючи із точки старту. Рівняння для перших семи кумулянтів розподілів втрат енергії у пружних, непружних та обох типах зіткнень розв'язані чисельно за допомогою методу, розвинутого авторами раніше, на інтервалі енергій іонів 1 кеВ–1 ГеВ. Їх порівняння з параметрами розподілу пробігів іонів показало, що: 1) середній шлях за розподілом втрат енергії становить 30–90% повного пробігу іонів; 2) при низьких енергіях страгглінг за розподілом втрат енергії дещо більший або однаковий із страгглінгом за розподілом пробігів іонів, а при високих енергіях перший перевищує останній у десятки разів; 3) скісності і ексцеси розподілів при низьких енергіях відповідно близькі, у той час як при високих енергіях їх зміна для розподілу втрат енергії на кілька порядків менша, ніж для розподілу пробігів іонів. Звідси випливає, що розподіл втрат енергії ширший і значно ближчий до нормального, ніж розподіл пробігів іонів при всіх енергіях імплантації. Показано, що ці властивості розподілу втрат енергії зумовлені новими членами у рівняннях, які не враховувалися раніше, але домінують при високих енергіях.