Solution of the kinetic equation for the deposited momentum distribution. II. Threshold energy effects

1995 J. Phys.: Condens. Matter 7 6365

(http://iopscience.iop.org/0953-8984/7/32/004)

J. Phys.: Condens. Matter 7 (1995) 6365–6377. Printed in the UK

Solution of the kinetic equation for the deposited momentum distribution: II. Threshold energy effects

L G Glazov

High-Current Electronics Institute, Akademichesky 4, Tomsk, Russia

Received 4 January 1995, in final form 12 April 1995

Abstract. The paper continues an investigation of the depth distribution of momentum deposited in solids by ion bombardment, finite-threshold-energy effects being discussed. It is shown that, for a wide set of system parameters, existing semianalytical techniques lead to a qualitatively incorrect description of momentum deposition, especially in the target surface region. The most important qualitative features of the deposited momentum distribution are considered, which cannot be ignored when finding solutions of the kinetic equation by analytically based methods or interpreting numerical simulation data. Corresponding analytical and numerical results are presented.

1. Introduction

The present paper is devoted to the depth distribution of momentum deposited in amorphous or polycrystalline targets by ion bombardment [1–6]. Although the results partly are qualitatively valid for more general approaches, the momentum deposition for simplicity is treated below for a relatively simple and well known model: an infinite isotropic random medium, neglecting electronic energy losses, power cross-section for elastic collisions $d\sigma(E, T) = CE^{-m}T^{-1-m}\,dT, 0 < m < 1$ [7–9, 4, 5], and equal masses of an ion and target atoms. We consider the distribution of the component of deposited momentum normal to the target surface; it is the most interesting function of the problem due to applications to the theory of sputtering [2–4, 10, 11] and its complicated behaviour [2, 5, 12, 6].

The present paper continues the work [12], wherein the deposited momentum distribution was investigated in assuming that the slowing down process can continue to arbitrary low particle energies via binary collisions between freely moving atoms. Including effects of atomic binding can be performed, as a first approximation, by introducing a finite threshold energy W defined as 'a minimum energy for a particle either to get displaced "permanently" from its original position or to displace other atoms' [9]. From a mathematical point of view, it is equivalent to the following boundary condition for the solutions of the kinetic equation:

$$\mathcal{P}(z, E, \eta) = (2ME)^{1/2}\eta\,\delta(z) \qquad \text{for } E \leqslant W \tag{1}$$

where z is a coordinate along the inner normal to the target surface, $z = 0$ at the surface; E, η, M are initial energy, direction cosine with respect to the z axis of velocity and mass of a projectile respectively; $\mathcal{P}(z, E, \eta)$ is the distribution to be found for $E > W$, $\mathcal{P}(z, E, \eta)\,dz$ being an average amount of momentum (z component) deposited in an interval $(z, z + dz)$.

The following circumstances have caused a special investigation of threshold energy effects. In the $m \leqslant \frac{1}{4}$ case, the deposited momentum distribution cannot at all be defined to be finite when neglecting threshold energy. For the $m > \frac{1}{4}$ region, although a solution of the kinetic equation exists in the $W = 0$ model, the $W > 0$ corrections are much greater than, for example, for the deposited energy or range distributions, and can hardly be neglected even for reasonable values $W/E \ll 1$. Moreover, as was pointed out in [12], for $W = 0$ the function $\mathcal{P}(z, E, \eta)$ has a specific singularity at $z = 0$, and, hence, the finite-W corrections near the target surface can even be of essentially larger order than ones in the rest of the distribution. Thus, correct analysis of momentum deposition near the target surface, being very important due to the sputtering theory applications, cannot be performed without introducing a finite threshold energy.

Although some analytical and numerical results will be presented below, this paper does not pretend to give the full and exact solution of the kinetic equation even for the simplified model being considered. First, it would be a rather complicated task; second, it is shown below that some parts of the solution in principle cannot be satisfactorily reconstructed by existing analytically based methods even for $W \ll E$. Moreover, the rough character of the model makes questionable the necessity of, say, exact tabulations of the solutions. So, the main attention is paid below to the most important *qualitative* features of the distribution, ignorance of which can lead (and often leads) to essentially incorrect calculations and understanding of characteristic behaviour of the deposited momentum profile, and which should be taken into account also for interpretation and interpolation of numerical simulation results.

2. Moment-like expansion of the distribution

Modifying the usual argument [8, 9] to take (1) into account, we have in the standard conventional notation the following integrodifferential equation for $\mathcal{P}(z, E, \eta)$:

$$-\eta \frac{\partial \mathcal{P}(z, E, \eta)}{\partial z} \theta(E - W) = N \int \mathrm{d}\sigma \{\mathcal{P} - \mathcal{P}' - \mathcal{P}''\} \tag{2}$$

where the second and third terms in the curly brackets represent the corresponding distributions for scattered and recoiling particles; $\theta(E) = 1$ for $E \geqslant 0$ and $= 0$ otherwise. The kinetic equation is completed by the momentum conservation condition, which determines the zeroth-order spatial moment of the distribution.

For $W = 0$ and $m > \frac{1}{4}$ [2, 12], the solution could be represented in the form

$$\mathcal{P}(z, E, \eta) = (2ME)^{1/2} NC/(3E^{2m}) F(zNC/E^{2m}, \eta). \tag{3}$$

The dimensionless function F has been tabulated in [12]. In the $W > 0$ case, the quantity E^{2m}/NC is no longer a universal length unit, since W^{2m}/NC has the dimension of a length also; the representation (3) is not valid and the solution can not be reduced to the function of two independent variables.

All the methods so far used for semianalytical calculation of the deposited momentum distribution are based upon reconstructing the function to be found from its spatial moments [2, 5, 12, 6]. So, in the present section we briefly consider the threshold energy corrections in the spatial moments, and discuss possibilities and limitations of the moments analysis approach.

For $W = 0, m > \frac{1}{4}$, the spatial moments $\mathcal{P}^n(E, \eta)$ of the distribution are as follows [12]:

$$\mathcal{P}^n(E, \eta) = \sum_l (2l + 1) P_l(\eta) \mathcal{P}_l^n(E) \qquad \mathcal{P}_l^n(E) = \frac{1}{3}(2ME)^{1/2} \left(\frac{E^{2m}}{NC}\right)^n F_l^n \tag{4}$$

where P_l are Legendre polynomials; F_l^n are the moments of the dimensionless function $F(x,\eta)$, introduced in (3), and are determined by the recurrence

$$\begin{aligned} F_l^n &= \frac{n[lF_{l-1}^{n-1} + (l+1)F_{l+1}^{n-1}]}{(2l+1)I_l(\frac{1}{2}+2mn)} \qquad n>0 \\ F_l^0 &= \delta_{l1} \end{aligned} \tag{5}$$

where†

$$I_l(s) = \int_0^1 t^{-1-m}\,\mathrm{d}t\left[1 - P_l(\sqrt{1-t})(1-t)^s - P_l(\sqrt{t})t^s\right].$$

For $E \gg W > 0$, including the case $m < \frac{1}{4}$, one can find the spatial moments by using the well known Laplace transformation method [14, 15, 9, 10, 11] (see also the appendix). This leads to asymptotic $W \ll E$ expansions for $\mathcal{P}_l^n$ in terms of some powers of W/E. The first terms are as follows:

$$\mathcal{P}_l^n(E) = \frac{1}{3}(2ME)^{1/2}\left(\frac{E^{2m}}{NC}\right)^n \left\{F_l^n + \left(\frac{W}{E}\right)^{2m-1/2}\mathcal{F}_l^n + \ldots\right\} \tag{6}$$

where $\mathcal{F}_l^n$ are determined by the recurrence

$$\begin{aligned} \mathcal{F}_l^n &= \frac{n[l\mathcal{F}_{l-1}^{n-1} + (l+1)\mathcal{F}_{l+1}^{n-1}]}{(2l+1)I_l(1+2m(n-1))} \qquad n>1 \\ \mathcal{F}_l^0 &= 0 \qquad \mathcal{F}_l^1 = \frac{\delta_{l0}}{(\frac{1}{2}-2m)I_0'(1)} \end{aligned} \tag{7}$$

while F_l^n still satisfy (5) both for $m > \frac{1}{4}$ and $m < \frac{1}{4}$.

For $m < \frac{1}{4}$ the second term in the curly brackets in (6) appears to be leading for $E \gg W$ (except $n = 0$, of course); for $m > \frac{1}{4}$ the relative $W > 0$ corrections in the moments of the deposited momentum distribution ($\sim (W/E)^{2m-1/2}$) are much greater than ones for the damage or range distributions, which are $\sim (W/E)^{2m+1/2}$ [9].

We will not analyse in detail the conditions which are necessary for the series (6) to be rapidly convergent; however, note one of them: $(W/E)^{4m} \ll 1$. Below, when discussing the $W/E \ll 1$ asymptotes of the solutions, we suppose that the ratio W/E is small enough for the few first terms in (6) to determine the spatial moments with good accuracy. In particular, the noted condition for pertinent values of W/E excludes too small values of m from the consideration.

Defining the function $\mathcal{F}(x,\eta)$ to have the moments $\mathcal{F}_l^n$, we can write the corresponding expansion for the distribution itself:

$$\mathcal{P}(z,E,\eta) = \frac{(2ME)^{1/2}NC}{3E^{2m}}\left\{F\left(\frac{zNC}{E^{2m}},\eta\right) + \left(\frac{W}{E}\right)^{2m-1/2}\mathcal{F}\left(\frac{zNC}{E^{2m}},\eta\right) + \ldots\right\}. \tag{8}$$

It can be immediately checked, by comparing (7) with analogous formulae in [9] or [13], that the function $\mathcal{F}(x,\eta)$ is proportional to the derivative of the $W = 0$ damage profile:

$$\mathcal{F}(x,\eta) = \frac{1}{(2m-\frac{1}{2})I_0'(1)}\frac{\mathrm{d}}{\mathrm{d}x}F^{(E)}(x,\eta) \tag{9}$$

† More precisely, the function $I_l(s)$ is defined by this integral only for $\mathrm{Re}\,s > m$; otherwise the analytical continuation is assumed; the latter can be easily obtained by expressing the integral in terms of the B function [9, 13].

where $F^{(E)}(x, \eta)$ is the deposited energy distribution for $W = 0$ in dimensionless variables ($F(x, \eta)$ in the notation of [13]).

The expansions (6),(8) give a clue to the only method used earlier in semianalytical investigations to calculate the deposited momentum profile. The method includes tabulation of a set of the moments taking into account a pertinent number of terms in the expansion (6), and forthcoming approximate reconstruction of the distribution from the moments (for example, by the Padé approximants technique). However, we are going to show below that this method, being very simple, useful, and informative, nevertheless fails for some cases and can lead (and had led) to qualitatively incorrect results. The sensitivity of the problem to the factors to be considered is different for relatively small values of m (roughly $m < \frac{1}{4}$) and large ones. So, we discuss these regions separately.

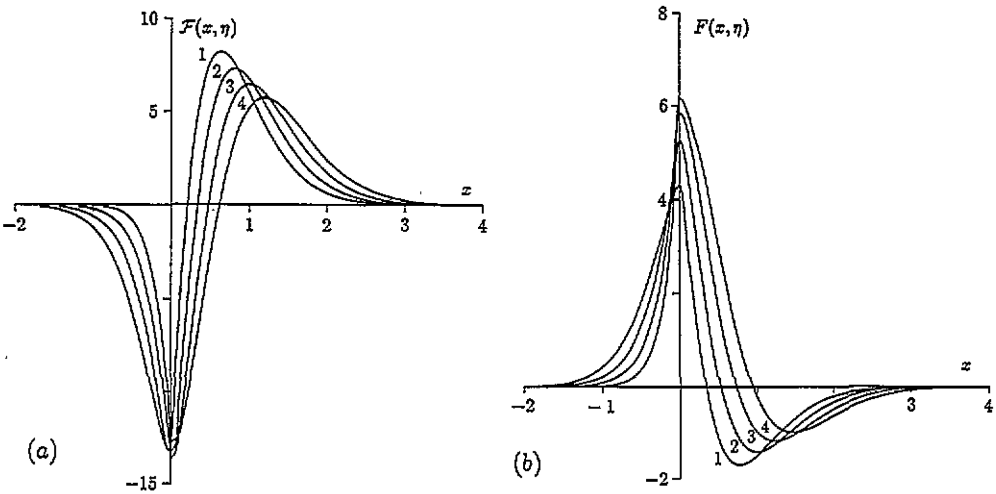

Figure 1. Two leading terms in the moment-like expansion (8) of the deposited momentum distribution: the functions $\mathcal{F}(x, \eta)$ (a) and $F(x, \eta)$ (b) for $m = \frac{1}{6}$; $\eta = 0.4$ (1), $\eta = 0.6$ (2), $\eta = 0.8$ (3), $\eta = 1$ (4).

For small values of m and $W \ll E$, the first two terms in the expansion (8) *really* can provide a good approximation for the whole distribution. Figure 1 demonstrates the behaviour of the functions $\mathcal{F}(x, \eta)$ and $F(x, \eta)$ for $m = \frac{1}{6}$ and a set of incidence angles. The method of tabulation is discussed in detail in [13, 12]. Figure 2 presents the whole distribution (with two terms in (8) taken into account) for $m = \frac{1}{6}$, $\eta = 1$ (normal incidence) and different values $W/E \ll 1$. In accordance with the physical sense of the deposited momentum distribution, it is positive and negative for large depths inside and outside the target respectively; the function is negative at the target surface; its absolute value decreases with growing W/E.

However, it is necessary to make the following note here. For moderately small values of W/E, when the first two terms in (8) do not provide any longer an appropriate accuracy, one could try to proceed by taking into account the next terms in the expansion (8) (or, equivalently, in (6)). It would be a fatal mistake, at least for calculating the distribution near the target surface, for the same reasons, which are discussed below in detail for the large-m case. Thus, we have the following alternative for the small-m region: either the ratio W/E is small enough for the two-term approximation to be valid (it is shown below that the respective criterion is $(W/E)^{1-3m} \ll 1$), or the method fails completely to calculate the distribution near the target surface.

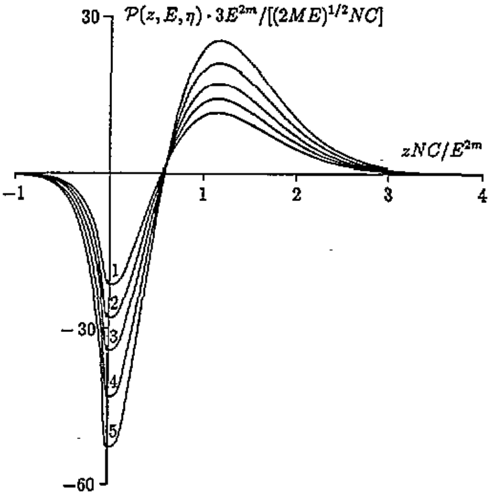

Figure 2. The deposited momentum distribution for normal incidence ($\eta = 1$); $m = \frac{1}{6}$; the two leading terms in the expansion (8) have been taken into account; the curves $1, \ldots, 5$ correspond to the values $W/E = 10^{-2}, 3 \times 10^{-3}, 10^{-3}, 3 \times 10^{-4}, 10^{-4}$.

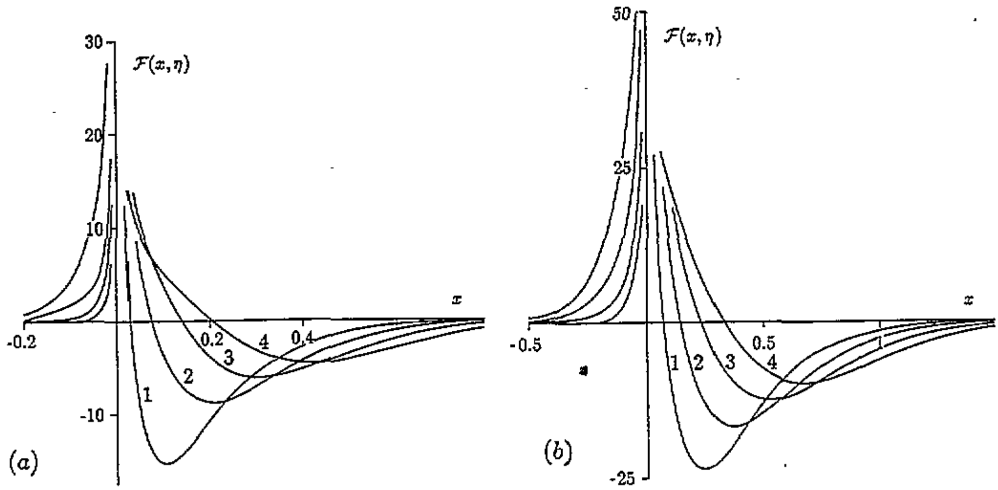

Figure 3. The leading threshold energy correction in the deposited momentum distribution for the large-m case: the function $\mathcal{F}(x, \eta)$; $m = \frac{1}{2}$ (a) and $m = \frac{1}{3}$ (b); $\eta = 0.4$ (1), $\eta = 0.6$ (2), $\eta = 0.8$ (3), $\eta = 1$ (4).

Consider now the relatively large-m case. For better understanding of the nature of difficulties appearing in this case, we begin from the concrete example. Suppose we want to calculate the distribution for $m = \frac{1}{3}$ (such calculations were made in [5] by the Padé approximants method) and some finite value of W/E, which is small enough to neglect all the terms in (6) except the first two. Suppose also that we have a very powerful computer and a very progressive scheme, allowing us to reconstruct a function *exactly* from its spatial moments. Then, after the calculation, we will find that the value of the distribution at the target surface is equal to infinity, because $\partial F^{(E)}/\partial x(x = 0) = \infty$ for $m = \frac{1}{3}$ [13].

Thus, when, taking into account the two first terms in (6), one obtains a finite value of the $W \neq 0$ correction in the distribution at the target surface; this finite value is determined *exclusively* by the degree of inaccuracy of the conventional scheme being used to reconstruct the function from its spatial moments, and has nothing to do with an actual value predicted by the kinetic equation. Moreover, even if an exact value of $\mathcal{P}(z=0)$ had been found *accidentally* for some fixed value of W/E, one inevitably would obtain a wrong result for another value of this ratio, because the formula (8) predicts an incorrect dependence of $\mathcal{P}(z=0)$ on W/E, as will be shown below.

So, the relation between the expansion (8) and the distribution to be found requires more detailed analysis. The function $F(x,\eta)$ has a singularity at the target surface, specified in [12], wherein the pertinent results of numerical tabulation are given also. The function $\mathcal{F}(x,\eta)$, calculated by the same method, is shown for $m=\frac{1}{2},\frac{1}{3}$ in figure 3(a, b). It is characterized by a stronger singularity for $x\to 0$ ($\sim|x|^{1/(2m)-3/2}$ for $m>\frac{1}{3}$ and $\sim\ln|x|$ for $m=\frac{1}{3}$). Thus, for example, the expression (8) in fact gives for fixed η, $E\gg W$ and $z\to 0$

$$\mathcal{P}=\frac{(2M)^{1/2}NC}{3E^{\frac{1}{6}}}\left[\{\text{constant}+\ldots\}+\left(\frac{W}{E}\right)^{\frac{1}{6}}\left\{\text{constant}\times\ln\left|\frac{zNC}{E^{2/3}}\right|+\ldots\right\}+\ldots\right]$$

$$\mathcal{P}=\frac{(2M)^{1/2}NC}{3E^{1/2}}\left[\left\{\text{constant}\times\ln\left|\frac{zNC}{E}\right|+\ldots\right\}\right.$$
$$\left.+\left(\frac{W}{E}\right)^{1/2}\left\{\text{constant}\times\left|\frac{zNC}{E}\right|^{-1/2}+\ldots\right\}+\ldots\right]$$

for $m=\frac{1}{3}$ and $m=\frac{1}{2}$ respectively. The expressions on the right-hand sides represent the first terms of the formal expansions of $\mathcal{P}$ in the region where such expansions are not valid†. Hence, the formula (8) is not correct in the thin target surface region, although it can give a reasonable approximation far away from $z=0$.

An attempt to improve the situation by taking into account a larger (but finite) number of terms in the expansion (8) would not be successful, since the next terms in (8) are characterized by stronger singularities for $z\to 0$, which do not compensate each other (at least while the full series has not been summed). Another method one could try—to introduce the finite-W corrections into each term separately, i.e., for example, redefine the second term to be proportional to the derivative of the deposited energy distribution taken for $W>0$—does not give serious advantages either, since it simply reduces the present problem to the problem on, say, the finite-W effects in the damage distribution's derivative, which is no simpler; moreover, the next terms in (8) being treated in the same way can give contributions of the same order to $\mathcal{P}(z=0)$.

Thus, calculations and understanding of characteristic features of the distribution near the target surface require an essentially different approach. It appears to be too difficult to give a detailed reconstruction of $\mathcal{P}(z,E,\eta)$ in the target surface region on the basis of existing analytical methods. However, for $\mathcal{P}(z=0)$ (which is especially important due to the sputtering theory applications), sufficiently full qualitative and even quantitative results can be obtained, and are considered in the next section and the appendix. Here one deals with two characteristic effects of great importance: a discontinuity of the distribution at the target surface, which has not been mentioned in this paper yet, and a specific dependence on energetic parameters for $W\ll E$, which, in particular, provides the failure of the moment-like expansion near the target surface.

† Note here a simple example of the function, which is finite and has a formal expansion similar to that for $m=\frac{1}{2}$, $z\to 0$: $\frac{1}{3}(2M)^{1/2}NCE^{-1/2}\ln\left[(|z|NC/E)^{1/2}+a(W/E)^{1/2}\right]f(zNC/E)$, where $a=\text{constant}>0$ and f is any smooth function, $f(0)\neq 0$.

3. The distribution at the target surface

3.1. The discontinuity of the distribution

The discontinuity of the distribution at the target surface in the infinite-medium model is a rather obvious effect from a physical point of view. It is determined by low-transfer-energy collisions of a projectile right after its start from the plane $z = 0$. Integrating the kinetic equation (2) over a small region including $z = 0$ taking (1) into account, we find for $E > W$

$$\begin{aligned} {}_\Delta\mathcal{P}(E,\eta) &\equiv \mathcal{P}(z=+0,E,\eta) - \mathcal{P}(z=-0,E,\eta) \\ &= (2M)^{1/2}E^{-1/2}N\left\{\int_{E-W}^{E}(E-T)\frac{\mathrm{d}\sigma(E,T)}{\mathrm{d}T}\,\mathrm{d}T + \int_0^W T\frac{\mathrm{d}\sigma(E,T)}{\mathrm{d}T}\,\mathrm{d}T\right\}. \end{aligned} \tag{10}$$

This formula is valid for arbitrary cross-section, including the case when electronic stopping is taken into account. For the power cross-section and $E > W$, we arrive at

$$\begin{aligned} {}_\Delta\mathcal{P}(E,\eta) = (2ME)^{1/2}NCE^{-2m}&\left[\frac{1}{1-m}\left(1-(1-W/E)^{1-m}\right)\right. \\ &\left.-\frac{1}{m}\left(1-(1-W/E)^{-m}\right)+\frac{1}{1-m}(W/E)^{1-m}\right]. \end{aligned} \tag{11}$$

For $E \gg W$, being $\sim(W/E)^{1-m}$, this discontinuity usually can be reasonably neglected. For example, it was not taken into account for calculations shown in figures 1, 2, and the terms (11) will not be rewritten in the formulae for the leading $W \ll E$ asymptotic terms in the next subsection. However, note here two cases when this discontinuity becomes very significant.

The first one is the case of almost tangential incidence of a projectile ($\eta \approx 0$). Really, ${}_\Delta\mathcal{P}$ is independent of η, while all other contributions into $\mathcal{P}(z = 0)$ are antisymmetric with respect to η. So, for tangential incidence $\mathcal{P}(z = \pm 0, E, \eta = 0) = \pm{}_\Delta\mathcal{P}/2$, and the discontinuity cannot be neglected for small enough values of η even for $W \ll E$.

The second case—moderately small values of W/E. Although formally the discontinuity represents the effect of lower order, quantitatively it can appear comparable with calculated values of the distribution at the target surface, especially for not very small m. As an example of what ignorance of the discontinuity can lead to, let us consider the results of [5], wherein the deposited momentum distribution was tabulated for $m = \frac{1}{3}$ and normal incidence ($\eta = 1$). The curve for the case $W/E = \frac{1}{10}$ ($E_1/E = \frac{1}{10}$ in the notation of [5]) indicates positive values of the distribution for $z \leqslant 0$. It is a very strange result from a physical point of view. Really, right after the beginning of the cascade the full momentum (z component) in the half-space $z < 0$, $p_{z<0} = 0$; during the cascade $p_{z<0}$ constantly decreases, because every particle penetrating the plane $z = 0$ either brings a negative amount of momentum in (if moving in negative direction), or takes a positive one out (otherwise). So, at least integrated over the region $z < 0$ deposited momentum must be negative. It is an ignorance of the discontinuity at the target surface that is mainly responsible for such a significant error, since for this case the formula (11) gives even larger ${}_\Delta\mathcal{P}$ than the value of $\mathcal{P}(z = 0)$ indicated in [5].

3.2. The $W \ll E$ asymptotes

In the present subsection we are going to consider a simple evaluation for finding the $E \gg W$ asymptote for $\mathcal{P}(z = 0)$. To be determined, the analytical evaluation is oriented to the case $m > \frac{1}{4}$, but the final result is valid as well for $m < \frac{1}{4}$. Being not very rigorous, this method does not use a complicated mathematical technique and can be applied with some restrictions for more realistic approximations for the cross-section, but it allows us to find only a very few terms in asymptotic expansions and does not give calculable expressions for some coefficients. A more complicated, regular method for finding asymptotic expressions for $\mathcal{P}(z=0)$ is discussed in the appendix.

Let us expand the distribution to be found in terms of Legendre polynomials with respect to angular dependence, analogously with (4), and use the notation

$$\Psi_l(E) = \int_0^\infty \mathcal{P}_l(z, E)\, \mathrm{d}z.$$

The functions $\mathcal{P}_l(z, E)$ satisfy the well known system of integrodifferential equations [9]. Integrating these equations over z, one expresses $\mathcal{P}_l(z=0, E)$ in terms of the functions $\Psi_l(E)$. A simple dimensional argument shows that Ψ_l can be represented in the form $\Psi_l(E) = \frac{1}{3}(2ME)^{1/2}\chi_l(W/E)$, where χ_l are dimensionless functions. For simplicity, we consider an example of finding the asymptotic expression for $\mathcal{P}_1(z=0, E)$, which can be expressed in terms of χ_l as follows:

$$\begin{aligned}\mathcal{P}_1(z=0, E)&\\ &= \frac{(2ME)^{1/2}NC}{3E^{2m}}\left\{\int_0^{1-W/E} t^{-1-m}\Big[\chi_0(W/E) - (1-t)^{1/2}\chi_0(W/E(1-t))\Big]\,\mathrm{d}t\right.\\ &\quad \left. - \int_{W/E}^1 t^{-1/2-m}\chi_0(W/Et)\,\mathrm{d}t - \chi_0(W/E)\Big[1-(1-W/E)^{-m}\Big]\right\}. \qquad (12)\end{aligned}$$

Although the functions χ_l are not known, some statements on their behaviour can be made. In accordance with the boundary condition (1), $\chi_l(1) = 0$ for $l \neq 1$. Being the spatial moments of the distribution, χ_l are continuous functions of W/E. The values $\chi_l(0)$ correspond to the solution in the $W=0$ case [12]: $\chi_l(0) = \int_0^\infty F_l(x)\,\mathrm{d}x$, $F_l(x)$ being the lth angular harmonics of $F(x,\eta)$. It was noted above that the relative corrections in all moments $\mathcal{P}_l^n$ are $\sim (W/E)^{2m-1/2}$ for $E \gg W$, so one can assume that the same is true for the functions χ_l:

$$\chi_l(W/E) \approx \chi_l(0) + \tilde{\chi}_l(W/E)^{2m-1/2} \qquad W \ll E \qquad (13)$$

where $\tilde{\chi}_l = \int_0^\infty \mathcal{F}_l(x)\,\mathrm{d}x \sim F_l^{(E)}(x=0)$. The validity of (13) can be shown more rigorously using the results of the appendix.

The last term in (12) is $\sim W/E$ and can be neglected. The first one is finite for $W/E \to 0$ and has the asymptotic expansion {constant + constant$\times (W/E)^{2m-1/2}$}, where the constants are expressed in terms of $\chi_0(0)$, $\tilde{\chi}_0$. It is the second integral in (12) that determines the difference between the orders of the $W > 0$ corrections in the spatial moments and in $\mathcal{P}_1(z=0, E)$. Let us examine this integral for $m = \frac{1}{2}$:

$$\begin{aligned}J \equiv -\int_{W/E}^1 t^{-1}\chi_0(W/Et)\,\mathrm{d}t&\\ &= -\int_{W/E}^1 \xi^{-1}\chi_0(\xi)\,\mathrm{d}\xi = -\chi_0(0)\ln(E/W) + \int_{W/E}^1 \xi^{-1}[\chi_0(\xi) - \chi_0(0)]\,\mathrm{d}\xi\\ &= -\chi_0(0)\ln(E/W) + \text{constant} + \text{constant} \times (W/E)^{2m-1/2} + \ldots.\end{aligned}$$

Making a similar evaluation for other m and l, after multiplying by $P_l(\eta)$ and summarizing on even l, we find the following three-term asymptote for $\mathcal{P}(z=0, E, \eta)$,

$W/E \ll 1$:

$$\mathcal{P}(z=0,E,\eta) = (2ME)^{1/2}NC/(3E^{2m}) \times \begin{cases} A_1(\eta)\ln(E/W) + A_2(\eta) + A_3(\eta)(W/E)^{1/2} + \ldots \\ \text{for } m = \frac{1}{2} \\ B_1^{(m)}(\eta) + B_2^{(m)}(\eta)(W/E)^{1/2-m} + B_3^{(m)}(\eta)(W/E)^{2m-1/2} + \ldots \\ \text{for } m \neq \frac{1}{4}, \frac{1}{3}, \frac{1}{2} \\ D_1(\eta) + D_2(\eta)(W/E)^{\frac{1}{6}}\ln(E/W) + D_3(\eta)(W/E)^{\frac{1}{6}} + \ldots \\ \text{for } m = \frac{1}{3}. \end{cases} \quad (14)$$

For $m \leqslant \frac{1}{2}$ the coefficients of the first terms are expressed via $F(x,\eta)$:

$$\left\{ \begin{array}{c} A_1(\eta) \\ B_1^{(m)}(\eta), D_1(\eta) \end{array} \right\} = \mp\frac{1}{\eta}\sum_{\text{even } l}(2l+1)P_l(\eta)\chi_l(0)\left\{ \begin{array}{c} P_l(0) \\ I_l(\frac{1}{2}) \end{array} \right\}. \quad (15)$$

For $\frac{1}{4} < m < \frac{1}{2}$, the expressions (15) for $B_1^{(m)}(\eta)$, $D_1(\eta)$, of course, can be easily obtained directly from the kinetic equation for $W = 0$. A similar representation was used in [13] to tabulate the deposited energy distribution at the target surface for $W = 0$, the effective numerical method of tabulating expressions of this kind being discussed also. The coefficients $A_3(\eta)$, $B_3^{(m)}(\eta)$, $D_2(\eta)$ can be similarly expressed in terms of the function $\mathcal{F}(x,\eta)$. The approach being discussed does not give calculable expressions for $A_2(\eta)$, $B_2^{(m)}(\eta)$, $D_3(\eta)$, because the expressions for these coefficients include integration of $\chi_l(\xi)$ over ξ in the interval (0,1). An alternative approach, giving a general method for finding calculable expressions for all coefficients, is discussed in the appendix. In principle, these formulae allow us to calculate an arbitrary number of coefficients in the asymptotic expansions (14); the corresponding results for the leading terms for $m = \frac{1}{2}$ and $m = \frac{1}{3}$ are demonstrated in figure 4(a, b). However, such calculations are very complicated, and it is difficult to reach high accuracy in some cases; moreover, the necessity of very accurate tabulations is questionable for the rough model being considered.

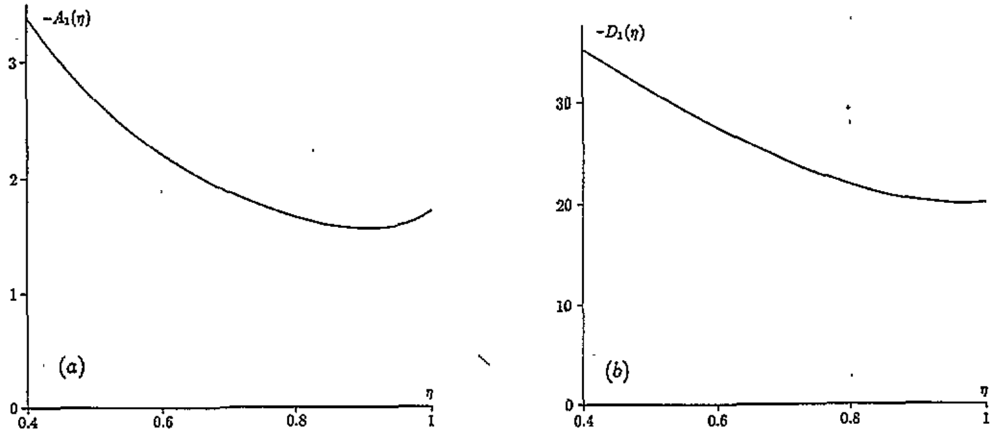

Figure 4. The large-m deposited momentum distribution at the target surface: the leading $W/E \ll 1$ asymptotic term coefficients $A_1(\eta)$ for $m = \frac{1}{2}$ (a) and $D_1(\eta)$ for $m = \frac{1}{3}$ (b) (see also the formula (14)) as functions of incidence angle cosine.

It would be a more interesting and important task to examine the qualitative features of the dependence of $\mathcal{P}(z=0)$ on energetic parameters. A competition of the three terms in the expansion (14) leads to essentially different dependences of the distribution at the target surface on energetic variables for different values of m (or, more generally, for different types of low-transfer-energy asymptote of the cross-section), and explains the failure of the moment-like expansion approach, which was discussed in the previous section. One can see that, in general, the asymptotic $W/E \ll 1$ expansion for $\mathcal{P}(z=0)$ contains some terms which do not appear in expansion (6) for the spatial moments.

For $m < \frac{1}{4}$, the third and first terms in (14) are the leading ones, and coincide with the first two terms of the moment-like expansion (8). The second term in (14) represents the largest subsequent correction (except, maybe, the case of very small m, when even the series for the spatial moments converges very poorly for reasonable values of W/E). It can be neglected for $(W/E)^{1-3m} \ll 1$; otherwise, one cannot proceed by taking into account additional terms in (8) either, and more sophisticated techniques (for example, the approach considered in the appendix) should be used for calculation.

From a formal point of view, a similar situation takes place also for $\frac{1}{4} < m < \frac{1}{3}$ (with the only restriction that in this case the finite $W=0$ solution can be obtained and the first term in (14) is largest for $W/E \to 0$); however, in practice the second term can hardly be neglected for any reasonable value of W/E, and the moment-like expansion (8) appears to be useless.

We have already shown in the previous section that the moment-like expansion approach fails for $m \geqslant \frac{1}{3}$. The formula (14) indicates the main reason for this: the finite-W corrections in $\mathcal{P}(z=0)$ ($\sim (W/E)^{1/6}\ln(E/W)$ and $\sim (W/E)^{1/2-m}$ for $m=\frac{1}{3}$ and $\frac{1}{3} < m < \frac{1}{2}$ respectively) are essentially larger than ones in the spatial moments ($\sim (W/E)^{2m-1/2}$). For $m \geqslant \frac{1}{2}$ no finite result can be found for $\mathcal{P}(z=0)$ in neglecting threshold energy, as shown earlier in the direct $W=0$ calculation [12]; the formula (14) indicates that for $m=\frac{1}{2}$ and $m > \frac{1}{2}$ the distribution at the target surface is characterized by logarithmic and power singularity respectively for $W/E \to 0$. The physical origin and characteristic features of this specific behaviour for relatively large m were discussed in detail in [12] for $W=0$; some estimations obtained appear useful. In particular, for the normal incidence case ($\eta=1$) and $m \geqslant \frac{1}{3}$, $\mathcal{P}(z=0)$ for $W=0$ can be roughly estimated as follows [12]:

$$\mathcal{P}(z=0, E, \eta=1) \approx -\beta_m N(2ME)^{1/2}\sigma_A(E) \tag{16}$$

where $\sigma_A(E) = \int_0^E (T/E)^{1/2}\,\mathrm{d}\sigma(E,T)$, $N(2ME)^{1/2}\sigma_A(E)$ being the average sum of absolute values of momenta of recoils created by a projectile per unit path length; $\beta_m = \frac{1}{3}\int_0^\infty F(x,\eta=0)\,\mathrm{d}x$. For $W \neq 0$, the analogous evaluation taking into account the cut-off of the cascade for $E < W$ leads again to the formula (16) with $\sigma_A(E) = \int_W^E (T/E)^{1/2}\,\mathrm{d}\sigma(E,T)$. The function $F(x,\eta=0)$ can be easily tabulated [12]; the respective values of β_m being $\beta_{1/2} \approx 1.7/3$, $\beta_{1/3} \approx 3.3/3$. For the power cross-section with $m=\frac{1}{3}$, $\sigma_A(E) = 6CE^{-2/3}[1-(W/E)^{1/6}]$ and the formula (16) gives ~5% error when used to estimate $D_1(\eta=1)$. For $m=\frac{1}{2}$, $\sigma_A(E) = CE^{-1}\ln(E/W)$ and the formula (16) gives an exact result for the leading asymptotic term, as can be easily verified by comparing (16) with (14), (15).

Acknowledgment

I wish to thank Professor P Sigmund for very useful discussions of the topic and his hospitality during my visit to Odense University.

Appendix. Laplace transformation method for finding distribution at the target surface

We are going to use a modification of the well known Laplace transformation method for finding the $W \ll E$ asymptotes for $\mathcal{P}(z = 0, E, \eta)$. The method was initially proposed for the Kinchin–Pease equation [14], and later was extensively applied for calculation of the spatial moments of the damage cascade theory distributions [15, 9–11]. The method is based on introducing a logarithmic variable $u = \ln(E/W)$ instead of E and the Laplace transformation with respect to u. A bar will be further used to denote Laplace transforms of the functions, for example: $\bar{\mathcal{P}}_l^n(s) \equiv \int_0^\infty \mathcal{P}_l^n(W e^u) e^{-su}\, du$. Laplace transformation being applied to the kinetic equation leads to the following recurrence relations for $\bar{\mathcal{P}}_l^n(s)$:

$$\begin{aligned} \bar{\mathcal{P}}_l^n(s+2m) &= \frac{W^{2m}}{NC} \frac{n\left[l\bar{\mathcal{P}}_{l-1}^{n-1}(s) + (l+1)\bar{\mathcal{P}}_{l+1}^{n-1}(s)\right]}{(2l+1)I_l(s+2m)} \qquad n \geqslant 1 \\ \bar{\mathcal{P}}_l^0(s) &= \frac{(2MW)^{1/2}\delta_{l1}}{3(s-\frac{1}{2})}. \end{aligned} \tag{A1}$$

Note here that the two-term asymptote (6) for the moments arises from the two major poles (at $s = \frac{1}{2} + 2mn$ and $s = 1 + 2m(n-1)$) of $\bar{\mathcal{P}}_l^n(s)$ calculated in accordance with (A1). It is convenient to introduce some new functions $G_l^n(s)$:

$$\bar{\mathcal{P}}_l^n(s) = \frac{(2MW)^{1/2}}{3(s - 2mn - \frac{1}{2})} \left(\frac{W^{2m}}{NC}\right)^n G_l^n(s - 2mn). \tag{A2}$$

Recurrence relations for $G_l^n(s)$ are local with respect to s.

Our local purpose is finding expressions for the Laplace transforms of the functions

$$\varphi_l(E) = \frac{1}{2l+1}\Big[l\mathcal{P}_{l-1}(z=0,E) + (l+1)\mathcal{P}_{l+1}(z=0,E)\Big].$$

The functions $\varphi_l(E)$ represent the angular harmonics of the function $\eta\mathcal{P}(z = 0, E, \eta)$. Excluding the terms connected with the discontinuity of the distribution at the target surface from the present consideration, we further suppose l to be even. Integrating the kinetic equation over z, after the Laplace transformation one can find

$$\bar{\varphi}_l(s) = NCW^{-2m} I_l(s+2m)\bar{\Psi}_l(s+2m) \tag{A3}$$

while the functions $\bar{\Psi}_l(s)$ can be expressed in terms of $G_l^n(s)$:

$$\bar{\Psi}_l(s) = -\frac{(2MW)^{1/2}}{3\pi i(s-\frac{1}{2})} \int_0^\infty \xi^{-1}\, d\xi \sum_{\text{odd } n} \frac{G_l^n(s)}{n!}(-i\xi)^n. \tag{A4}$$

Let us define the functions $G_l(s|x)$ as a set of solutions of the following system of equations:

$$\begin{aligned} -\frac{\partial}{\partial x}&[lG_{l-1}(s|x) + (l+1)G_{l+1}(s|x)] \\ &= (2l+1)\int_0^1 t^{-1-m}\, dt\Big[G_l(s|x) - P_l(\sqrt{1-t})(1-t)^{s-2m}G_l(s|x/(1-t)^{2m}) \\ &\quad - P_l(\sqrt{t})t^{s-2m}G_l(s|x/t^{2m}) - \delta(x)G_l^0(s) \\ &\quad \times[1 - P_l(\sqrt{1-t})(1-t)^s - P_l(\sqrt{t})t^s]\Big] \end{aligned} \tag{A5}$$

with the normalization condition

$$G_l^0(s) \equiv \int_{-\infty}^{\infty} G_l(s|x)\,\mathrm{d}x = \delta_{l1}. \tag{A6}$$

It is easy to check that the functions $G_l^n(s)$ coincide with the spatial moments of the functions $G_l(s|x)$. For any fixed s, the system (A5), (A6) is essentially similar to ones for different $W = 0$ damage cascade distributions in dimensionless variables. For example, the deposited momentum $W = 0$ problem [12] is a special case of (A5), (A6) with $s = \frac{1}{2}$: $F_l(x) \equiv G_l(\frac{1}{2}|x)$. The deposited energy distribution $W = 0$ problem [13] is a special case of (A5) with $s = 1$, when the normalization condition $G_l^0 = \delta_{l0}$ is used instead of (A6). For other fixed values of s, the system (A5), (A6) in principle can be solved by the method which was discussed in detail in [13, 12]. Thus, any functionals, including the functions $G_l(s|x)$ with fixed s, can be considered as known values.

The sum on the right-hand side of (A4) represents the Fourier transform of the function $G_l(s|x)$ with respect to x, so the integral can be rewritten in the form

$$-\frac{1}{\pi\mathrm{i}}\int_0^{\infty} \xi^{-1}\,\mathrm{d}\xi \sum_{\text{odd } n} \frac{G_l^n(s)}{n!}(-\mathrm{i}\xi)^n = \int_0^{\infty} G_l(s|x)\,\mathrm{d}x \equiv G_l^{(0)}(s).$$

In particular, for $s = \frac{1}{2}$ we have $G_l^{(0)}(\frac{1}{2}) = \chi_l(0)$. Now we can rewrite the formula (A3) as follows:

$$\bar{\varphi}_l(s) = \frac{NC(2MW)^{1/2}}{3W^{2m}(s + 2m - \frac{1}{2})} I_l(s + 2m) G_l^{(0)}(s + 2m). \tag{A7}$$

The leading $W \ll E$ asymptotic terms in backward Laplace transforms are obtained by calculating contributions of a few first poles of $\bar{\varphi}_l(s)$. The three major poles are as follows:

(i) $s_1 = \frac{1}{2} - 2m$—provides the $W = 0$ result, if it is finite ($\frac{1}{4} < m < \frac{1}{2}$);
(ii) $s_2 = -m$—the first pole of $I_l(s + 2m)$;
(iii) $s_3 = 1 - 4m$—the first root of the equation $I_0(s + 4m) = 0$, determining the first pole of $G_l^{(0)}(s + 2m)$ in accordance with (A1), (A2).

Contributions of these poles give the three-term expansions (14), the coefficients being expressed in terms of the values $G_l^{(0)}(s)$ at $s = s_j$ and, maybe, some associated functions.

For $m \neq \frac{1}{2}, \frac{1}{3}, \frac{1}{4}$ all the poles are simple, and contributions of the poles are $\sim W^0$, $W^{1/2-m}$, $W^{2m-1/2}$ in agreement with (14). Consider, for example, the contributions of two leading poles for $\frac{1}{3} < m < \frac{1}{2}$ and $m > \frac{1}{2}$:

$$\varphi_l(E) \approx \frac{NC(2ME)^{1/2}}{3E^{2m}} \left\{ I_l(\tfrac{1}{2})\chi_l(0) + \left(\frac{W}{E}\right)^{1/2-m} \frac{P_l(0)G_l^{(0)}(m)}{\frac{1}{2} - m} \right\}.$$

Multiplying by $(2l + 1)P_l(\eta)$ and summarizing on even l, we find the expressions for the coefficient functions $B_1^{(m)}(\eta)$ and $B_2^{(m)}(\eta)$, the former being the same as in (15), and

$$B_2^{(m)}(\eta) = \frac{1}{(\frac{1}{2} - m)\eta} \sum_{\text{even } l} (2l + 1) P_l(\eta) P_l(0) G_l^{(0)}(m).$$

The values $m = \frac{1}{2}, \frac{1}{3}$ are characterized by the presence of the second-order poles, which lead to appearing logarithmic factors in the respective terms of backward Laplace transforms. Being a bit more complicated than in the previous case, the evaluation is straightforward and expresses the coefficients in (14) in terms of $G_l^{(0)}(s = s_j)$ and $(\mathrm{d}/\mathrm{d}s)G_l^{(0)}(s = s_j)$.

References

[1] Littmark U 1974 *Thesis* University of Copenhagen
[2] Littmark U and Sigmund P 1975 *J. Phys. D: Appl. Phys.* **8** 241
[3] Sigmund P 1977 *Inelastic Ion–Surface Collisions* ed N H Tolk *et al* (New York: Academic) p 121
[4] Sigmund P and Sckerl M W 1993 *Nucl. Instrum. Methods* B **82** 242
[5] Roosendaal H E, Littmark U and Sanders J B 1982 *Phys. Rev.* B **26** 5261
[6] Sckerl M W, Vicanek M and Sigmund P 1995 *Nucl. Instrum. Methods* B at press
[7] Lindhard J, Nielsen V and Scharff M 1968 *K. Danske Vidensk. Selsk. Mat.-Fys. Meddr.* **36** No 10
[8] Lindhard J *et al* 1963 *K. Danske Vidensk. Selsk. Mat.-Fys. Meddr.* **33** No 10
[9] Winterbon K B, Sigmund P and Sanders J B 1970 *K. Danske Vidensk. Selsk. Mat.-Fys. Meddr.* **37** No 14
[10] Sigmund P 1969 *Phys. Rev.* **184** 383
[11] Falcone D 1990 *Riv. Nuovo Cimento* **13** 1
[12] Glazov L G 1994 *J. Phys.: Condens. Matter* **6** 10647
[13] Glazov L G 1994 *J. Phys.: Condens. Matter* **6** 4181
[14] Robinson M T 1965 *Phil. Mag.* **12** 145
[15] Sigmund P 1969 *Radiat. Eff.* **1** 15