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On the differentiability of depth distribution function of deposited energy, momentum and ion range*

a reply to Dr L. G. Glazov

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Based on the translational invariance of a medium, a new theorem has been proposed and proved rigorously: the depth distributions of the deposited energy, momentum and ion range must be infinitely differentiable functions in amorphous or polycrystalline infinite targets by ion bombardment, if these functions exist. The origin of the "discontinuity", derived by Dr Glazov in 1995 in J. Phys.: Condens. Matter **7** 6365, has been analysed in detail. For the power cross section, neglecting electronic stopping, the linear transport equations determining the depth distribution functions of the deposited energy and momentum (by taking the threshold energy into account) have been solved asymptotically. An important formula derived by Dr Glazov has been confirmed and generalized. The results agree with the new theorem.

Keywords: Radiation damage, momentum deposition, ion implantation
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1. Introduction

The depth distribution functions of the deposited energy, momentum and ion range have been studied by several authors.[1−8] Part of reason is that the energy and momentum deposited at the target surface are related to the sputtering phenomenon.[3,4,9,13] However, these distribution functions have never been proved rigorously to be continuous and differentiable, only it is postulated to be so from the physics points of view. From 1994 to 1995, Dr Glazov demonstrated the "singularity" or "discontinuity" of these functions at the target surface.[10−12] Thus, a collection of analytical works[1−8] has turned out to be questionable.

Recently, the author of this paper published a "comment"[14] to refute these arguments.[10−12] Soon, Dr Glazov published a reply[15] to the "comment".[14] Since the "singularity" derived in Refs.[10] and [11] has been refuted based on its violation of the Parseval's identity in Ref.[14], the present paper mainly focuses on the continuity and differentiability of the above-mentioned distribution functions, as a reply to Dr Glazov's reply.[15]

2. Differentiability of depth distribution functions of deposited energy, momentum and ion range

The depth distributions of the deposited energy $F_D(z,\boldsymbol{\nu})$ (momentum $\boldsymbol{P}_D(z,\boldsymbol{\nu})$) and the ion range $F_R(z,\boldsymbol{\nu})$, as a consequence of a projectile slowing-down from velocity $\boldsymbol{\nu}$ (or energy E) at the surface z=0 in an amorphous or polycrystalline infinite medium, are defined so that $F_D(z,\boldsymbol{\nu})\mathrm{d}z$ (momentum $\boldsymbol{P}_D(z,\boldsymbol{\nu})\mathrm{d}z$) and $F_R(z,\boldsymbol{\nu})\mathrm{d}z$ are, respectively, the average amounts of energy (momentum) and probability of the projectile located in a layer $(z,\mathrm{d}z)$, after the projectile and recoiling (not for the ion range) atoms have slowed down below a certain threshold $E \geq W > 0$. The case of neglecting threshold energy[9,10] can be considered as a limit ($W \to 0$) of the case $W > 0$,[11] if the limit exists. For $E > W$, to the first order in δz, and using the translational invariance of the medium,[1] $H_{(i)}(z,\boldsymbol{\nu})$ must satisfy

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$$H_{(i)}(z,\boldsymbol{\nu}) = N\delta z \int \mathrm{d}\sigma[H_{(i)}(z,\boldsymbol{\nu}') + \delta_{i1}H_{(i)}(z,\boldsymbol{\nu}'')] + (1 - N\sigma\delta z)H_{(i)}(z - \eta\delta z, \boldsymbol{\nu}), \quad (1)$$

where i=0,1. $H_0(z,\boldsymbol{\nu})$ represents $F_R(z,\boldsymbol{\nu})$ and $H_1(z,\boldsymbol{\nu})$ represents one of $F_D(z,\boldsymbol{\nu})$ and $\boldsymbol{P}_D(z,\boldsymbol{\nu})$. z is the coordinate along the inner normal to the target surface, M and N are atomic mass and atomic number density of the target respectively, and η is the cosine of incident angle, $1 \geq \eta > 0$. $\mathrm{d}\sigma = \mathrm{d}\sigma(\boldsymbol{\nu};\boldsymbol{\nu}';\boldsymbol{\nu}'')$ is the differential cross section for scattering between an atom moving with velocity $\boldsymbol{\nu}$ and an atom at rest. $\boldsymbol{\nu}'$ and $\boldsymbol{\nu}''$ represent the velocities of the scattered and recoiling atoms respectively; the integrations are taken over all possible (binary) collisions. The total cross section is $\boldsymbol{\sigma} \equiv \int \mathrm{d}\sigma$=finite, because, $N\sigma\delta z$ appears in Eq.(1) as a probability (less than unity). The case of $\sigma = \infty$ can be considered as a limit ($\sigma \to \infty$) of the case σ=finite, if $\lim\limits_{\sigma\to\infty} H_{(i)}(z,\boldsymbol{\nu})$ exists.

Theorem. $H_{(i)}(z,\boldsymbol{\nu})$ determined by Eq.(1) is a continuous and infinitely differentiable function of z, in both cases σ=finite and $\sigma = \infty$ if it exists.

Proof. The critical point is that Eq.(1) was derived based on σ=finite. The solution of Eq.(1) may be extended to a case $\sigma = \infty$. But, in the case $\sigma = \infty$, δz approaching zero ($\delta z \to 0$) in Eq.(1) must be executed first, and $\sigma \to \infty$ second to guarantee against the occurrence of $N\sigma\delta z \to \infty$. Since σ=finite, $H_{(i)}(z,\boldsymbol{\nu})$ is finite and

$$\int \mathrm{d}\sigma[H_{(i)}(z - \eta\delta z, \boldsymbol{\nu}) - H_{(i)}(z,\boldsymbol{\nu}') - \delta_{i1}H_{(i)}(z,\boldsymbol{\nu}'')] = (\text{finite quantity}).$$

Thus the discontinuity of $H_{(i)}(z,\boldsymbol{\nu})$ is determined by

$$\lim_{\sigma\to\infty}\lim_{\delta z\to 0}[H_{(i)}(z - \eta\delta z,\boldsymbol{\nu}) - H_{(i)}(z,\boldsymbol{\nu})] = N\lim_{\delta\to\infty}\lim_{\delta z\to 0}[\delta z \cdot (\text{finite quantity})] = 0. \quad (2)$$

So $H_{(i)}(z,\boldsymbol{\nu})$ must be a continuous function of z in both cases σ=finite and $\sigma = \infty$. For σ=finite, one can see $H^{(1)}_{(i)}(z,\boldsymbol{\nu})$=finite, where

$$H^{(0)}_{(i)}(z,\boldsymbol{\nu}) \equiv H_{(i)}(z,\boldsymbol{\nu}) \text{ and } H^{(n)}_{(i)}(z,\boldsymbol{\nu}) \equiv \frac{\partial^2 H_{(i)}(z,\boldsymbol{\nu})}{\partial z^n}, \quad n = 1,2,3,\cdots$$

Assuming that $H^{(n-1)}_{(i)}(z,\boldsymbol{\nu})$ is finite for σ=finite, to the first order in $\mathrm{d}z$, and using the translational invariance of the medium,[1] $H^{(n-1)}_{(i)}(z,\boldsymbol{\nu})$ must satisfy

$$H^{(n-1)}_{(i)}(z - \eta\delta z,\boldsymbol{\nu}) - H^{(n-1)}_{(i)}(z,\boldsymbol{\nu}) = N\delta z \int \mathrm{d}\sigma[H^{(n-1)}_{(i)}(z - \eta\delta z,\boldsymbol{\nu}) - H^{(n-1)}_{(i)}(z,\boldsymbol{\nu}') - \delta_{i1}H^{(n-1)}_{(i)}(z,\boldsymbol{\nu}'')]. \quad (3)$$

The same argument results in that $H^{(n-1)}_{(i)}(z,\boldsymbol{\nu})$ must be a continuous function of z in both cases σ=finite and $\sigma = \infty$. For σ=finite, one can see $H^{(n)}_{(i)}(z,\boldsymbol{\nu})$=finite. Therefore, $H_{(i)}(z,\boldsymbol{\nu})$ must be infinitely differentiable with respect to z in both cases σ=finite and $\sigma = \infty$, if it exists. This completes the proof.

Expanding the second term on the right-hand side of Eq.(1) to the first order in $\mathrm{d}z$, one obtains the basic linear transport equations determining $H_{(i)}(z,\boldsymbol{\nu})$.

$$-\eta\partial H_{(i)}(z,\boldsymbol{\nu})/\partial z = N\int \mathrm{d}\sigma[H_{(i)}(z,\boldsymbol{\nu}) - H_{(i)}(z,\boldsymbol{\nu}') - \delta_{i1}H_{(i)}(z,\boldsymbol{\nu}'')], \quad (4)$$

which is obviously equivalent to Eq.(1) if and only if the right-hand side is finite. The space moments of $H_{(i)}(z,\boldsymbol{\nu})$ defined by

$$H^n_{(i)}(z,\boldsymbol{\nu}) = \int_{-\infty}^{\infty} \mathrm{d}z \cdot z^n H_{(i)}(z,\boldsymbol{\nu}) = \sum_{L=0}^{\infty}(2L+1)H^n_{(i)L}(E)P_L(\eta), \quad n = 0,1,2,3,\cdots$$

obey the following recursion relations

$$\begin{cases} nLH^{n-1}_{(i)L-1}(E) + n(L+1)H^{n-1}_{(i)L+1}(E) \\ = (2L+1)N\int_0^E \mathrm{d}\sigma(E,T)[H^n_{(i)L}(E) \\ \quad - P_L(\sqrt{1-T/E})H^n_{(i)L}(E-T) \\ \quad - \delta_{i1}P_L(\sqrt{T/E})H^n_{(i)L}(T)], \\ H^n_{(i)L}(T \leq W) = 0, \quad n = 1,2,3,\cdots \end{cases} \quad (5)$$

The great success of Eq.(4) has made many authors take it for granted that Eq.(4) is equivalent to Eq.(1) for $\sigma = \infty$.[1-8] As a matter of fact, this allegation may not always be true. Based on Eq.(5) and the normal condition (n=0), one can see that if

$$\frac{\mathrm{d}\sigma(E,T\neq 0)}{\mathrm{d}T} = \text{finite} \quad \text{and} \quad S_n(E) \equiv \int_0^E \mathrm{d}\sigma(E,T)T = \text{finite}, \quad (6)$$

the space moments of $F_R(z,\boldsymbol{\nu})$ are finite for $W \geq 0$ and those of $H_{(i)}(z,\boldsymbol{\nu})$ are finite for $W > 0$, thus $H_{(i)}(z,\boldsymbol{\nu})$ can exist. According to the new theorem,

$H_{(i)}(z,\boldsymbol{\nu})$ must be a continuous and infinitely differentiable function of z under the corresponding condition. Since the condition (6) is always satisfied in the traditional theoretical model,[1,3] the "discontinuity" derived by Glazov[12] is nothing but a mathematical illusion.

In order to search for the origin of the "discontinuity",[12,15] it is necessary to restudy $P_D(z,\boldsymbol{\nu})$ (the perpendicular component of $\boldsymbol{P}_D(z,\boldsymbol{\nu})$).

For $E<W$, if σ=finite one should have a trivial depth distribution function

$$P_D(z,\boldsymbol{\nu})=\eta\sqrt{2ME}\cdot f(z,\sigma), \tag{7}$$

$$f(z,\sigma)\equiv\begin{cases}(N\sigma/\eta)\exp(-zN\sigma/\eta), & \text{for } z\geq 0,\\ 0, & \text{for } z<0.\end{cases} \tag{8}$$

If $\sigma=\infty$ Eq.(8) turns out to be a delta function, and Eq.(7) reduces to

$$P_D(z,\boldsymbol{\nu})=\eta\sqrt{2ME}\cdot\delta(z). \tag{9}$$

For $E>W>0$ a collision cascade will be initiated. For cascades not too dense, $P_D(z,\boldsymbol{\nu})$ obeys Eqs.(4) and (7),[1,2] or

$$\begin{cases}-\eta\partial P_D(z,\boldsymbol{\nu})/\partial z\\ =N\displaystyle\int_0^E \mathrm{d}\sigma[P_D(z,\boldsymbol{\nu})-P_D(z,\boldsymbol{\nu}')-P_D(z,\boldsymbol{\nu}'')],\\ P_D(z,\boldsymbol{\nu})=\eta\sqrt{2ME}\cdot f(z,\sigma), \quad \text{for } E<W.\end{cases} \tag{10}$$

Equation (10) can be written as

$$\begin{aligned}&-\frac{\eta}{N}\cdot\frac{\partial P_D}{\partial z}\\ =&Q(z,E,\eta)-(2M)^{0.5}f(z,\sigma)\\ &\times\left[\int_{E-W}^{E}\mathrm{d}\sigma\eta'\sqrt{E-T}+\int_0^W\mathrm{d}\sigma\eta''\sqrt{T}\right],\end{aligned} \tag{11}$$

where

$$\begin{aligned}Q(z,E,\eta)\equiv&\int_0^E\mathrm{d}\sigma P_D(z,E,\eta)\\ &-\int_0^{E-W}\mathrm{d}\sigma P_D(z,E-T,\eta')\\ &-\int_W^E\mathrm{d}\sigma P_D(z,T,\eta'').\end{aligned}$$

Considering that each term on the right-hand side of Eq.(11) is finite in the case of σ=finite, integrating Eq.(11) over a small region $a>z>-a$ yields

$$\begin{aligned}&\lim_{\sigma\to\infty}\{\lim_{a\to 0}[\Delta P_D(e,\eta)]\}\\ \equiv&P_D(z=+0,E,\eta)-P_D(z=-0,E,\eta)=0.\end{aligned}$$

So, $P_D(z,\boldsymbol{\nu})$ has absolutely no "jump" at z=0 for the conditional arbitrary cross section (6). This conclusion confirms the previous theorem. In contrast, integrating $f(z,\sigma)$ over a small region $a>z>-a$, Glazov has obtained

$$\lim_{a\to 0}\left[\lim_{\sigma\to\infty}\int_{-a}^{a}\mathrm{d}zf(z,\sigma)\right]=\lim_{a\to 0}\int_{-a}^{a}\mathrm{d}z\delta(z)=1,$$

which obviously violates the translational invariance of the medium.[1] This violation resulted in the "discontinuity" of $P_D(z,\boldsymbol{\nu})$ at z=0.[12,15]

In 1996, Sckerl *et al.*[6] performed Monte Carlo simulations for $P_D(z,\boldsymbol{\nu})$ in accordance with the same theoretical model characterized by the power cross section. Although the cut-off impact parameter used for the simulation is large enough to ensure a negligible systematic error, it is still finite in practice, thus $P_D(z,\boldsymbol{\nu})$ should satisfy Eq.(11) and must be a continuous infinitely differentiable function of z. A very strange "non-zero jump" of $P_D(z,\boldsymbol{\nu})$ demonstrated by Fig.3 in Ref.[6] for E/W=10 was probably caused by the poor depth resolution.

3. Depth distribution functions of deposited-momentum and energy for the power cross section

For the power cross section $\mathrm{d}\sigma(E,T)=CE^{-m}T^{-1-m}\mathrm{d}T$ $(1>m>0)$ and $W>0$, Sigmund *et al.*[1,2,6] have found that $F_D(z,\boldsymbol{\nu})$ and $P_D(z,\boldsymbol{\nu})$ satisfy simple scaling laws, and can be represented in the forms

$$\begin{cases}F_D(z,\boldsymbol{\nu})=NCE^{1-2m}F(x,w,\eta),\\ P_D(z,\boldsymbol{\nu})=\dfrac{1}{3}(2M)^{0.5}NCE^{0.5-2m}P(x,w,\eta),\end{cases} \tag{12}$$

where $x\equiv zNC/E^{2m}$, $w\equiv W/E$. $F(x,w,\eta)$ and $P(x,w,\eta)$ can be expanded as

$$\begin{aligned}F(x,w,\eta)=&F_{(0)}(x,\eta)-w^{2m+0.5}\\ &\times[F_{(1)}(x,\eta)-w^{2m-0.5}\cdot F_{(2)}(x,\eta)]+\cdots,\\ P(x,w,\eta)=&[P_{(0)}(x,\eta)-w^{2m-0.5}\cdot P_{(1)}(x,\eta)]\\ &-w^{4m}\cdot[P_{(2)}(x,\eta)-w^{2m-0.5}\\ &\cdot P_{(3)}(x,\eta)]+\cdots.\end{aligned}$$

The space moments of dimensionless function $U(x,w,\eta)$ can be expanded as

$$\begin{aligned}U^n(w,\eta)=&\int_{-\infty}^{\infty}\mathrm{d}x\cdot x^nU(x,w,\eta)\\ =&\sum_{L=0}^{\infty}(2L+1)U_L^n(w)P_L(\eta),\end{aligned}$$

where U represents one of $F, P, F_{(\mu)}$ and $P_{(\mu)}$. The expansion coefficients are given by

$$F_L^n(w) = F_{(0)L}^n - w^{2m+0.5} \cdot [F_{(1)L}^n - w^{2m-0.5} \cdot F_{(2)L}^n] + \cdots$$

$$P_L^n(w) = [P_{(0)L}^n - w^{2m-0.5} \cdot P_{(1)L}^n] - w^{4m} \cdot [P_{(2)L}^n - w^{2m-0.5} \cdot P_{(3)L}^n] + \cdots$$

$F_{(0)L}^n$ and $P_{(0)L}^n$ were given in Refs.[10]–[12]. Other coefficients are

$$F_{(1)L}^n = \alpha_1 \cdot nP_{(0)L}^{n-1}, \quad P_{(1)L}^n = \beta_1 \cdot nF_{(0)L}^{n-1}, \qquad n \geq 2;$$

$$F_{(2)L}^n = \alpha_2 \cdot nP_{(1)L}^{n-1}, \quad P_{(2)L}^n = \beta_2 \cdot nF_{(1)L}^{n-1}, \qquad n \geq 3;$$

$$P_{(3)L}^n = \beta_3 \cdot nF_{(2)L}^{n-1}, \qquad n \geq 4.$$

The constants α_μ are β_ν defined as

$$\alpha_1 = \frac{(1-m)\Gamma_m}{3(2m+0.5)},$$

$$\alpha_2 = 2(2m-0.5)\left[\frac{1}{(-4m)}F_{(0)1}^1 + \frac{1}{(2m-0.5)}F_{(1)1}^1\right];$$

$$\beta_1 = \frac{(1-m)\Gamma_m}{(2m+0.5)},$$

$$\beta_2 = 2(2m+0.5) \cdot \left[\frac{P_{(0)0}^1 + 2P_{(0)2}^1}{4m} + \frac{P_{(1)0}^1}{(2m+0.5)}\right];$$

$$\beta_3 = \frac{3(1-m)\Gamma_m}{\alpha_2} \times \left[\frac{P_{(0)1}^2}{6m-0.5} + \frac{P_{(1)1}^2}{4m} + \frac{P_{(2)1}^2}{(2m-0.5)}\right];$$

Substituting these coefficients into Eqs.(12), one obtains

$$F(x,w,\eta) = F_{(0)}(x,\eta) + w^{2m+0.5} \cdot [\alpha_1 \partial P_{(0)}(x,\eta)/\partial x] + w^{2m-0.5} \cdot (\alpha_2\beta_1)\partial^2 F_{(0)}(x,\eta)/\partial x^2] + \cdots, \quad 1 \gg w > 0, \tag{13}$$

$$P(x,w,\eta) = [P_{(0)}(x,\eta) + w^{2m-0.5} \cdot \beta_1 \partial F_{(0)}(x,\eta)/\partial x] - w^{4m} \cdot [(\alpha_1\beta_2)\partial^2 P_{(0)}(x,\eta)/\partial x^2 + w^{2m-0.5} \cdot (\alpha_2\beta_1\beta_3)\partial^3 F_{(0)}(x,\eta)/\partial x^3] + \cdots, \quad 1 \gg w > 0. \tag{14}$$

Taking the first bracket on the left-hand side of Eq.(14) only, one can obtain Dr Glazov's formula (Eq.(8) in Ref.[12]), which has been derived by Dr Glazov correctly and quoted later by Sigmund.[6]

Since $U(x,w,\eta)$ are continuous and infinitely differentiable functions, $\partial^n U_{(0)}(x,y)/\partial x^n$ must be finite functions, i.e. $U_{(0)}(x,\eta)$ must be infinitely differentiable functions of x, if it exists. In contrast, if $U_{(0)}(x,\eta)$ has any "singularity" or "discontinuity", $U(x,w,\eta)$ cannot be infinitely differentiable functions of x. This conclusion confirms the theorem in section 2.

4. Summary

(1) A new theorem has been proposed and proved: the depth distributions of the deposited energy, momentum and ion range must be infinitely differentiable functions of the depth, if they exist. The existence conditions of these distribution functions have been discussed in some detail.

(2) For the power cross section, the linear transport equations determining the space moments of $F_D(z,\boldsymbol{\nu})$ and $P_D(z,\boldsymbol{\nu})$ have been solved exactly for W=0 and asymptotically for $W > 0$. The conclusion confirms the new theorem.

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