

# THEORY OF DIELECTRIC FUNCTION AND STOPPING POWER IN INHOMOGENEOUS MANY-ELECTRON SYSTEMS

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We calculate the stopping power for planar channeled ions by use of the method of an inhomogeneous dielectric function. In an inverse inhomogeneous dielectric function, the density gradient effect appears. Such an effect contributes to the weak dependence of the stopping power on impact parameter from the channel wall. We also derive not only the stopping power formula for the system that the electron density has an axial symmetry, but also the formula in which higher order terms of the inverse dielectric function are taken into account, using the method of decoupling.

## 1. Introduction

In 1964, the quantum mechanical analysis of the stopping power due to the dielectric function's method was performed by Lindhard and Winter under the system of free electron gas<sup>1</sup>. By introducing the local density approximation (LDA) to the above formula, various kind of theoretical calculations of the stopping power were performed<sup>2</sup>. LDA was phenomenologically proposed in order to analyze the inhomogeneous electronic systems from the statistical point of view<sup>3</sup>. The dielectric theory of inhomogeneous many-electron systems is a new and challenging field<sup>4,5</sup>. Lundqvist<sup>6</sup> and Lozovik et.al.<sup>7</sup> reviewed the framework of the general theory on dielectric function for inhomogeneous many-electron systems. The framework of the general theory of the dielectric function  $\epsilon^{6,7}$  is expressed as follows

$$\epsilon(r_1, r_2, \omega) = \sigma(r_1 - r_2) - \int \Pi(r_1, r_3, \omega) v_e(r_3 - r_2) dr_3, \quad (1)$$

where  $v_e(r_3 - r_2) = e^2 / |r_3 - r_2|$  is Coulomb interaction between electrons.  $\Pi$  is a polarization operator and is also expressed by the following equation

$$\Pi(r_1, r_3, \omega) = \frac{1}{\hbar} \sum_{j,k} p_j(r_1, r_3) p_k(r_3, r_1) \frac{\Theta(E_F - E_k) - \Theta(E_F - E_j)}{\omega + \hbar^{-1}(E_k - E_j) + i\eta} \quad (2)$$

In the above,  $p_j$  and  $\Theta$  are the  $j$ -th element of density matrix and Heaviside step function, respectively.  $E_F$  and  $E_j$  are Fermi energy and the eigen energy of the  $j$ -th electron.  $\eta$  denotes the positive infinitesimal.

In 1986, under the high frequency response, we derived the first order analytical formulae of dielectric and inverse dielectric functions,  $\epsilon$  and  $\epsilon^{-1}$ , in inhomogeneous systems of many electrons, and showed the theoretical interpretation of LDA<sup>8</sup>.  $\epsilon$  and  $\epsilon^{-1}$  in inhomogeneous system are given by

$$\begin{aligned} \epsilon(r_1, r_2, \omega) &= \delta(r_1 - r_2) + \frac{1}{m\omega^2} \text{div}_{r_1} \left( n(r_1) \text{grad}_{r_1} \frac{e^2}{|r_1 - r_2|} \right) \\ &= \delta(r_1 - r_2) \left( 1 - \frac{\omega_p^2(r_1)}{\omega^2} \right) - \frac{e^2(r_1 - r_2)}{m\omega^2 |r_1 - r_2|^3} \text{grad}_{r_1} n(r_1), \end{aligned} \quad (3)$$

$$\epsilon^{-1}(r_1, r_2, \omega) \cong \frac{\omega^2}{\omega^2 - \omega_p^2(r_1)} \left( \delta(r_1 - r_2) - \frac{e^2}{m\omega^2 - \omega_p^2(r_2)} \frac{1}{|r_1 - r_2|^3} \text{grad}_{r_1} n(r_1) \right). \quad (4)$$

Here,  $n(r_1)$  is the electron density, and  $r_1$  and  $r_2$  are position vectors of electron and projectile, respectively. In eqs.(3) and (4),  $\omega_p$  is the plasma frequency which is defined due to the electron density  $n$  and mass  $m$  as follows

$$\omega_p^2(r_1) = \frac{4\pi e^2 n(r_1)}{m} \quad (5)$$

As a convenience, we express a complex variable ( $= \omega + i\eta$ ) as  $\omega$  in eqs.(3) and (4). Therefore,  $\varepsilon$  and  $\varepsilon^{-1}$  are complex and have real and imaginary parts.

In 1988, we also derived the general formula for stopping power for a system in which the electron distribution is possible to be treated to change one-dimensionally<sup>9</sup>. An arbitrary function of electron density is included in our formula. Our formula was successfully applied to analyze the stopping power at the surface<sup>10</sup>. In 1993, we also showed that eq.(3) is derived not only from the quantum mechanical standpoint of view, but also from the classical one<sup>11</sup>.

In this work, using our general formula, we calculate the stopping power for planar channeled ions, and showed the weak dependence of the stopping power on impact parameter from the channel wall<sup>12</sup>, we also derive the stopping power formula for the system that the electron density has the axial symmetry, and derive the fundamental formula in which higher order contributions are taken into account by use of the method of decoupling.

## 2. Stopping Power for Planar Channeling

The definition of the stopping power due to electromagnetism is given by

$$S = -Z_1 e \text{grad } r_1 \cdot \left. \frac{\partial \varphi(r_1, t_1)}{\partial t_1} \right|_{r_1=r_2} \frac{V}{V} \quad (r_b = (b(Vt_1))), \quad (6)$$

where  $Z_1 e$ ,  $V$  and  $b$  are the charge, the velocity and the impact parameter of projectile,  $\varphi$  is the dynamical polarization potential in which a bare Coulomb field  $\varphi_c$  is subtracted.  $\varphi$  is represented as the following equation

$$\varphi(r_1, t_1) = \varphi(r_1, t_1) - \varphi_c(|r_{11} - b|, z_1 - Vt_1) \quad (\varphi_c(r_1 - r_2) = \frac{Z_1 e}{|r_1 - r_2|}). \quad (7)$$

In eq. (7),  $\varphi$  is the dynamical polarization potential which is expressed by use of  $\varepsilon^{-1}$  in  $r_1 - \omega$  space as follows

$$\varphi(r_1, \omega) = \int dr_2 dr_3 \varphi_c(|r_1 - r_3|) \varepsilon^{-1}(r_3, r_2, \omega) \rho^{\text{ext}}(r_2, \omega). \quad (8)$$

In the above,  $\rho^{\text{ext}}$  is the number density of projectile in  $r - \omega$  space. If we take the classical straight path of projectile,  $\rho^{\text{ext}}$  becomes

$$\rho^{\text{ext}}(r_2, \omega) = \frac{1}{V} \delta(r_2 - b) e^{i\omega z_2 / V}. \quad (9)$$

The formula for stopping power  $S(b)$  for the system, in which the electron density  $n(x)$  is possible to be treated to change one-dimensionally and perpendicularly to the projection of an incident ion, is given as follows<sup>9</sup> (10)

$$S(b) = \frac{(Z_1 e)^2}{V^2} \left( \omega_p^2(b) \int_0^{q_{\text{max}}} \frac{dq_y}{\sqrt{q_y^2 + (\omega_p(b)/V)^2}} - \frac{1}{2} \int dx_3 \frac{\partial \omega_p^2(x_3)}{\partial x_3} \frac{b - x_3}{|b - x_3|} P \frac{1}{\omega_p^2(b) - \omega_p^2(x_3)} \right) \times \\ \left( \omega_p^2(b) \int_0^{q_{\text{max}}} \frac{dq_y}{\sqrt{q_y^2 + (\omega_p(b)/V)^2}} e^{-2|x_3 - b| \sqrt{q_y^2 + (\omega_p(b)/V)^2}} - \omega_p^2(x_3) \int_0^{q_{\text{max}}} \frac{dq_y}{\sqrt{q_y^2 + (\omega_p(x_3)/V)^2}} e^{-2|x_3 - b| \sqrt{q_y^2 + (\omega_p(x_3)/V)^2}} \right)$$

Here we take the propagating direction of the projectile as  $z$ -axis.  $b$  and  $x$  are the impact parameter of the projectile from the channel wall and the position coordinate along  $x$ -axis, respectively.  $q$  and  $q_{\max}$  are a wave number and a maximum one corresponding to the Fourier components over  $y$ -axis.  $P(\cdot \cdot \cdot)$  indicates the principal value.

Fujii et al. successfully applied our formula to analyze the position-dependent stopping power at surfaces of  $NaCl$ -type crystals<sup>10</sup>. In planar channeling case, we use the following Molière electron density

$$n(x_3) = \frac{Z_2 B}{2\sigma_c} \left( 0,35e^{-B|x_3|} + 2,2e^{-4B|x_3|} + 2e^{-20B|x_3|} \right), \quad (11)$$

where  $B = 0,3 / a_{TF}$  and  $\sigma_c = 1 / (2LN_c) \cdot a_{TF}$ ,  $L$  and  $N_c$  are the Thomas-Fermi screening length, the half distance between planar plane and the density of lattice atom, respectively.

Using  $S(b)$  given by eq.(10), we obtain the stopping power  $S(X)$  for planar channeling given in eq.(12)

$$S(X) = \sum_{i=-n}^{i=n} (S(iL - X) + S(iL + X)). \quad (12)$$

In the above,  $X$  is the distance from the midpoint of the planar channel. We take  $n = 5$  in performing numerical calculations.

In fig.1, for 3MeV  $He$  ions in the  $Au(111)$  channel, we show numerical results which is normalized at the midpoint of the planar channel ( $X = 0$ ).  $S, S_B$  and  $S_R$  denote the results for  $S = S_B + S_N$ ,  $S_B$  only and Robinson's phenomenological analysis, respectively. We use  $S_R$  which is given as follows

$$S_R(X) = S_0 + S_1 \sigma(X), \quad \sigma(X) = \frac{d}{dX} \sqrt{\frac{2}{V_p'(0)} (V_p(X) - V_p(0))}, \quad (13)$$

where  $V_p(X)$  denotes the planar continuum potential derived from Molière model<sup>13</sup>.

Deviations between  $S$  and  $S_B$  appear over the whole range of the planar channel, which mean that contributions of  $S_N$  to  $S$  are effective in our case. At the well defined channeling region, agreements between ours and Robinson's one are good. In such a region,  $S_N$  gives the weak dependence of the stopping power on impact parameter, which is caused by contributions due to distant collisions. Deviations appear as the projectile approaches to the channel wall. If we take into account of the random stopping power, it is rather reasonable that the rapid increase appears in  $S$  than  $S_R$  at the neighborhood of the channel wall.

### 3. Stopping Power for Axial Case

In this chapter, we derive the formula of stopping power for axial case in which the electron density of the many-electron system has the axial symmetry. In this case, taking into account that the function of electron density becomes  $n(r_\perp)$ , we can obtain the following stopping power  $S(b)$  from eqs.(4) and (6)~(9)

$$S(b) = \frac{i(Z_1 e)^2}{2\pi^2 V^2} \int_{-\infty}^{\infty} d\omega \omega \int dq_\perp \frac{1}{q_\perp^2 + (\omega/V)^2} \int dr_\perp e^{-iq_\perp(b-r_\perp)} \left( \varepsilon(r_\perp, b, \frac{\omega}{V}, \omega) - \delta(r_\perp - b) \right)_{\text{complex}} \quad (14)$$

In the above,  $b$  is the impact parameter from the string of lattice atoms. Performing the following integration in eq. (14)

$$\int dq_{\perp} \frac{1}{q_{\perp}^2 + (\omega/V)^2} e^{-iq_{\perp}(b-r_{\perp})} = 2\pi \int_0^{q_{\perp \max}} dq_{\perp} \frac{q_{\perp}}{q_{\perp}^2 + (\omega/V)^2} J_0(q_{\perp}|b-r_{\perp}|), \quad (15)$$

we have

$$S(b) = \frac{i(Z_1 e)^2}{\pi V^2} \int_{-\infty}^{\infty} d\omega \omega \int_0^{q_{\perp \max}} dq_{\perp} \frac{q_{\perp}}{q_{\perp}^2 + (\omega/V)^2} \int dr_{\perp} J_0(q_{\perp}|b-r_{\perp}|) \left( \varepsilon(r_{\perp}, b, \frac{\omega}{V}, \omega) - \delta(r_{\perp} - b) \right) \quad (16)$$

where  $J_0$  is the Bessel function of the zeroth order, and  $q_{\perp \max}$  corresponds to the maximum momentum transfer in two dimensional  $q_{\perp}$  space perpendicular to the direction of z-component.

From eq.(4) and the gradient in cylindrical coordinate  $(r_{\perp}, \theta, z)$

$$\text{grad } n = \frac{\partial n}{\partial r_{\perp}} e_{r_{\perp}} + \frac{1}{r_{\perp}} \frac{\partial n}{\partial \theta} e_{\theta} + \frac{\partial n}{\partial z} e_z, \quad (17)$$

and taking into account of the axial symmetry of electron density  $n$ , we have the following result after performing Foulter transformation aver z-axis

$$\begin{aligned} \left( \varepsilon(r_{\perp}, b, \frac{\omega}{V}, \omega) - \delta(r_{\perp} - b) \right)_{\text{complex}} &= \left( \frac{\omega_p^2(r_{\perp})}{\omega^2 - \omega_p^2(r_{\perp})} \right)_{\text{complex}} \delta(r_{\perp} - b) - \\ &- \frac{e^2}{m} \left( \frac{\omega^2}{\omega^2 - \omega_p^2(r_{\perp})} \frac{1}{\omega^2 - \omega_p^2(b)} \right)_{\text{complex}} \frac{2(b \cos \theta - r_{\perp}) |\omega|}{|b - r_{\perp}| V} K_1 \left( |b - r_{\perp}| \frac{|\omega|}{V} \right) \frac{\partial n(r_{\perp})}{\partial r_{\perp}} \end{aligned} \quad (18)$$

where  $K_1$  is the modified Bessel function of the second kind. In eq. (17),  $e_{r_{\perp}}, \dots$  are unit vectors of cylindrical coordinate.

In eq.(18), imaginary parts of  $(\dots)_{\text{complex}}$  are expressed as follows

$$\Im \left( \frac{\omega_p^2(b)}{\omega^2 - \omega_p^2(b)} \right)_{\text{complex}} = -\frac{\pi}{2} \omega_p(b) \left( \delta(\omega - \omega_p(b)) - \delta(\omega + \omega_p(b)) \right). \quad (19)$$

$$\begin{aligned} \Im \left( \frac{\omega^2}{\omega^2 - \omega_p^2(r_{\perp})} \frac{1}{\omega^2 - \omega_p^2(b)} \right)_{\text{complex}} &= -\frac{\pi}{2} P \left( \frac{1}{\omega_p^2(r_{\perp}) - \omega_p^2(b)} \right) \\ &\times \left( \omega_p(r_{\perp}) \left( \delta(\omega - \omega_p(r_{\perp})) - \delta(\omega + \omega_p(r_{\perp})) \right) - \omega_p(b) \left( \delta(\omega - \omega_p(b)) - \delta(\omega + \omega_p(b)) \right) \right) \end{aligned} \quad (20)$$

Substituting eqs. (18)~(20) to eq. (16), we can obtain  $S(b)$ . Taking into account that  $S(b)$  is dependent only on  $b$ , we express the stopping power as  $S$ . Therefore, we have

$$S = S_B + S_N \quad (21)$$

$$S_B = \frac{(Z_1 e)^2}{V^2} \omega_p^2(b) \log \frac{\sqrt{q_{\perp \max}^2 + (\omega_p(b)/V)^2}}{\omega_p(b)/V}, \quad (22)$$

$$\begin{aligned}
S_N = & -\frac{(Z_1 e)^2}{2\pi V^2} \int dr_{\perp} \frac{(b \cos \theta - r_{\perp})}{|b - r_{\perp}|} \frac{\partial \omega_{\rho}^2(r_{\perp})}{\partial r_{\perp}} P \left( \frac{1}{\omega_{\rho}^2(r_{\perp}) - \omega_{\rho}^2(b)} \right) \\
& \times \left( \frac{\omega_{\rho}^3(r_{\perp})}{V} F \left( |b - r_{\perp}|, \left( \frac{\omega_{\rho}(r_{\perp})}{V} \right)^2, q_{\perp \max} \right) K_1 \left( |b - r_{\perp}| \frac{\omega_{\rho}(r_{\perp})}{V} \right) \right. \\
& \left. - \frac{\omega_{\rho}^3(b)}{V} F \left( |b - r_{\perp}|, \left( \frac{\omega_{\rho}(b)}{V} \right)^2, q_{\perp \max} \right) K_1 \left( |b - r_{\perp}| \frac{\omega_{\rho}(b)}{V} \right) \right)
\end{aligned} \tag{23}$$

In eq. (23),  $F$  is defined by the following equation

$$F \left( |b - r_{\perp}|, \left( \frac{\omega_{\rho}}{V} \right)^2, q_{\perp \max} \right) = \int_b^{q_{\perp \max}} dq_{\perp} \frac{q_{\perp}}{q_{\perp}^2 + (\omega/V)^2} J_0(q_{\perp} |b - r_{\perp}|). \tag{24}$$

If we take as  $q_{\perp \max}^2 + (\omega_{\rho}(b)/V)^2 = (2mV/\hbar)^2$  in eq. (22), we have

$$S_B = \frac{(Z_1 e)^2}{V^2} \omega_{\rho}^2(b) \log \frac{2mV^2}{\hbar \omega_{\rho}(b)}, \tag{25}$$

which is corresponding to the usual Bethe formula. Also if we take as  $q_{\perp \max} \rightarrow \infty$  in eq. (24), we obtain

$$F \left( |b - r_{\perp}|, \left( \frac{\omega_{\rho}}{V} \right)^2, q_{\perp \max} = \infty \right) = K_0 \left( |b - r_{\perp}| \frac{|\omega|}{V} \right). \tag{26}$$

Then, eq.(23) reduces to the following equation

$$\begin{aligned}
S_N = & -\frac{(Z_1 e)^2}{2\pi V^2} \int dr_{\perp} \frac{(b \cos \theta - r_{\perp})}{|b - r_{\perp}|} \frac{\partial \omega_{\rho}^2(r_{\perp})}{\partial r_{\perp}} P \left( \frac{1}{\omega_{\rho}^2(r_{\perp}) - \omega_{\rho}^2(b)} \right) \\
& \times \left( \frac{\omega_{\rho}^3(r_{\perp})}{V} K_0 \left( |b - r_{\perp}| \frac{\omega_{\rho}(r_{\perp})}{V} \right) K_1 \left( |b - r_{\perp}| \frac{\omega_{\rho}(r_{\perp})}{V} \right) - \right. \\
& \left. - \frac{\omega_{\rho}^3(b)}{V} K_0 \left( |b - r_{\perp}| \frac{\omega_{\rho}(b)}{V} \right) K_1 \left( |b - r_{\perp}| \frac{\omega_{\rho}(b)}{V} \right) \right)
\end{aligned} \tag{27}$$

In case of the high and nonrelativistic velocity region, we can approximate

$$K_0 \left( |b - r_{\perp}| \frac{\omega_{\rho}(u)}{V} \right) \cong \log \frac{2V}{|b - r_{\perp}| \omega_{\rho}(u)} - \gamma = \log \frac{2V}{\chi |b - r_{\perp}| \omega_{\rho}(u)}, \tag{28}$$

$$K_1 \left( |b - r_{\perp}| \frac{\omega_{\rho}(b)}{V} \right) \cong \frac{V}{|b - r_{\perp}| \omega_{\rho}(u)}, \tag{29}$$

where  $\gamma = 0.5772$  is Euler constant, and  $\chi = e^{\gamma} = 1.7812$ . Therefore, we obtain the formula which corresponds to such a velocity region under the boundary condition that  $\omega_{\rho}^2(\infty) = 0$

$$S_A = \frac{(Z_1 e)^2}{V^2} \left( \omega_\rho^2(b) \left( \log \frac{\chi^{b\omega_\rho}(b)}{2V} + \xi \right) + \frac{1}{2} \left( \int_0^b dr_\perp - \int_0^\infty dr_\perp \right) \frac{\partial \omega_\rho^2(r_\perp)}{\partial r_\perp} \log \left( 1 - \left( \frac{r_\perp}{b} \right)^2 \right) \right), \quad (30)$$

where  $\xi = \pi^2 / 12 - 1 / 2 = 0,3225$

In fig.2 and fig.3, we show numerical results of the stopping power for 10 and 50MeV  $H$  ions as a function of  $b$  from the  $Au \langle 100 \rangle$  string. Under the reasonable condition,  $S_A$  is more convenient than  $S_N$  because numerical computing times are shorter in  $S_A$  than in  $S_N$ . We confirm that the simplified formula  $S_A$  approaches to  $S_N$  as the incident energy of  $H$  becomes higher. In comparison between  $S_B$  and  $S_N$ ,  $S_N$  has the weaker dependence on  $b$  than  $S_B$ . Such a dependence is the same effect with the one-dimensional case which is coming from distant collisions, as is already mentioned in chapter 2. It is an important point that as distances from the axial string become larger than a few  $\text{\AA}$ ,  $S_N$  becomes more dominant, process than  $S_B$ . Recently, Fujii *et.al*, performed experiments to analyze string effects of the position-dependent stopping power<sup>14</sup>. In order to analyze such effects, it should be necessary to use the formula which is derived in this chapter.

#### 4. Iteration of Higher Order Terms

Under the high frequency approximation,  $\Pi$  given in eq.(2) is expanded by  $1/\omega$  as follows

$$\Pi(r_1, r_3, \omega) = \sum_{n=0}^{\infty} \frac{(-1)^n}{(\hbar\omega)^{n+1}} T_n(r_1, r_3) \quad (\omega \leftarrow \omega + i\eta), \quad (31)$$

$$T_n(r_1, r_3) = \sum_{j,k} (E_k - E_j)^n \rho_j(r_1, r_3) \rho_k(r_3, r_1) (\Theta(E_F - E_k) - \Theta(E_F - E_j)) \quad (32)$$

If there is no total current in the system of many electrons, odd power parts of  $1/\omega$  disappear. In such a case, we can take into account of even power parts only in  $\Pi$ . Then we have

$$\begin{aligned} \Pi(r_1, r_3, \omega) &= \sum_{j,k} (E_k - E_j) \rho_j(r_1, r_3) \rho_k(r_3, r_1) (\Theta(E_F - E_k) - \Theta(E_F - E_j)) \\ &\times \left( \sum_{n=1}^{\infty} \frac{(E_k - E_j)^{2(n-1)}}{(\hbar\omega)^{2n}} \right) \end{aligned} \quad (33)$$

In eq. (33), performing that the term  $(E_k - E_j)^2$  is replaced by the mean value  $\langle (E_k - E_j)^2 \rangle$ , we obtain

$$\sum_{n=1}^{\infty} \frac{\langle (E_k - E_j)^2 \rangle^{(n-1)}}{(\hbar\omega)^{2n}} = \frac{1}{\hbar^2 \omega^2} \sum_{n=0}^{\infty} t^n = \frac{1}{\hbar^2 \omega^2} \frac{1}{1-t} = \frac{1}{\hbar^2 (\omega^2 - \omega_j^2)}, \quad (34)$$

where  $\omega_j^2 = \langle (E_k - E_j)^2 \rangle / \hbar^2$ ,  $t = \omega_j^2 / \omega^2$ . Such a kind replacement corresponds to the decoupling usually used in Green's function. Therefore, we have  $\Pi$

$$\Pi(r_1, r_3, \omega) = \frac{1}{\hbar^2 (\omega^2 - \omega_j^2)} \sum_{j,k} (E_k - E_j) \rho_j(r_1, r_3) \rho_k(r_3, r_1) (\Theta(E_F - E_k) - \Theta(E_F - E_j)). \quad (35)$$

By use of the expression of eq.(35), we can use the same sum-rule by which we derive the basic equation of  $\varepsilon$  shown in eq.(3)<sup>8,9</sup>. Then, we have the following equations of  $\varepsilon$  and  $\varepsilon^{-1}$  in which higher order terms are taken into account through  $\omega_j$

$$\begin{aligned}\varepsilon(r_1, r_2, \omega) &= \delta(r_1 - r_2) + \frac{1}{m(\omega^2 - \omega_l^2)} \operatorname{div}_{r_1} \left( n(r_1) \operatorname{grad}_{r_1} \frac{e^2}{|r_1 - r_2|} \right) \\ &= \delta(r_1 - r_2) \left( 1 - \frac{\omega_p^2(r_1)}{\omega^2 - \omega_l^2} \right) - \frac{e^2}{m} \frac{1}{(\omega^2 - \omega_l^2)} \frac{(r_1 - r_2)}{|r_1 - r_2|^3} \operatorname{grad}_{r_1} n(r_1),\end{aligned}\quad (36)$$

$$\varepsilon^{-1}(r_1, r_2, \omega) \approx \frac{\omega^2 - \omega_l^2}{\omega^2 - (\omega_p^2(r_1) + \omega_l^2)} \left( \delta(r_1 - r_2) - \frac{e^2}{m} \frac{1}{\omega^2 - (\omega_p^2(r_2) + \omega_l^2)} \frac{(r_1 - r_2)}{|r_1 - r_2|^3} \operatorname{grad}_{r_1} n(r_1) \right) \quad (37)$$

As is wellknown, elementary excitation energies are expressed through poles about  $\omega$  in  $\varepsilon^{-1}$ . Therefore, by taking into account of the iteration of higher order terms, excitation energies are given by  $\hbar\sqrt{\omega_p^2(r_{1,2}) + \omega_l^2}$  in eq.(37) although they are given by  $\hbar\omega_p(r_1)$  in eq.(4). Effects of bound states of electrons are included in  $\omega_l$ . In order to show the usefulness of eq.(37), we try to calculate  $\hbar^2\omega_l^2$  for the case of the free electron gas system. In the free electron gas system, the mean value  $\hbar^2\omega_l^2$  is defined and derived as follows

$$\begin{aligned}\hbar^2\omega_l^2 &= \frac{3}{4\pi q_f^3} \int_{q_l \leq q_f} dq_j (E_k - E_j)^2 \\ &= \frac{3}{4\pi q_f^3} \frac{\hbar^4}{4m^2} \int_{q_l \leq q_f} dq_j (k^4 + 4q_j k^3 \cos\theta + 4q_j^2 k^2 \cos^2\theta) \\ &= \frac{\hbar^4}{m^2} \left( \frac{k^4}{4} + \beta_c^2 k^2 \right) \quad \left( \beta_c^2 = \frac{q_f^2}{5} \right),\end{aligned}\quad (38)$$

where  $\hbar\beta_c/m$  is the phase velocity of plasmon based on the classical model (as is usually known<sup>15</sup>, in case of quantum mechanics, we have  $\beta_q^2 = 3q_f^3/5$ ). In eq.(38), the terms proportional to  $k^4$  and  $k^2$  correspond to the single electron excitation and the dispersion relation of plasmon, respectively. Therefore, in case of the free electron gas, we can obtain, from eqs.(37) and (38), the exactly same energy expression<sup>15</sup> of elementary excitation  $I_e$ .

$$I_e^2 = \hbar^2\omega_p^2 + \frac{\hbar^4\beta_c^2 k^2}{m^2} + \frac{\hbar^4 k^4}{4m^2}. \quad (39)$$

Then, from the mathematical standpoint of view, we show the usefulness of the decoupling given in eq.(34), and also confirm that through  $\omega_l$  defined here, we can take into account of binding effects of electrons in inhomogeneous many-electron systems.

## 5. Concluding Remarks

In this work, using basic equations of  $\varepsilon$  and  $\varepsilon^{-1}$  given by eqs.(3) and (4)<sup>8,9</sup>, we derive stopping power formula for planar channeling as one-dimensional case, which was successfully used for the case of surface<sup>10</sup>. Numerical calculations of the stopping power for planar channeling were performed for the case of 3McV He ions into the Au {111} channel. Comparisons between theoretical and experimental results were also performed, and we obtained qualitative agreements between them. The weak dependence of the stopping power on impact parameter was typically caused by distant collisions. Such kind effects are not taken into account in the usual Bethe-type theory.

In two-dimensional case, the stopping power formula in inhomogeneous system was constructed under the condition of the cylindrical symmetry of electron density. We performed numerical calculations for cases of 10 and 50 MeV H ions in the Au,  $\langle 100 \rangle$  string. As is same with one-dimensional case, we also confirm important contributions of distant collisions. Recently, Fujii et.al. performed experiments to analyze string effects of the position-dependent stopping power<sup>14</sup>. In order to analyze such effects, it should be necessary to use the formula discussed here.

Using the decoupling method in Green's function, we took into account of the iteration of higher order contributions, and derived general formulae of the dielectric function and the inverse dielectric function. Applying such formulae to the case of the free electron gas, we obtained the exactly same dispersion relation of the free electron gas, in which terms of phase velocity of plasmon and single electron excitations appear. From the mathematical standpoint of view, we show the usefulness of the decoupling, and also confirm that through  $\omega_p$ , we can generally take into account of binding effects of electrons in inhomogeneous many-electron systems.

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## Figure Captions

Fig.1 Numerical calculations of the stopping power for planar channeling as a function of  $X$  for 3 MeV He ions in the Au  $\{111\}$  channel.

Fig.2 Numerical calculations of the stopping power as a function of  $b$  for 10 MeV H ions from the Au  $\langle 100 \rangle$  string.

Fig.3 Numerical calculations of the stopping power as a function of  $b$  for 50 MeV H ions from the Au  $\langle 100 \rangle$  string.



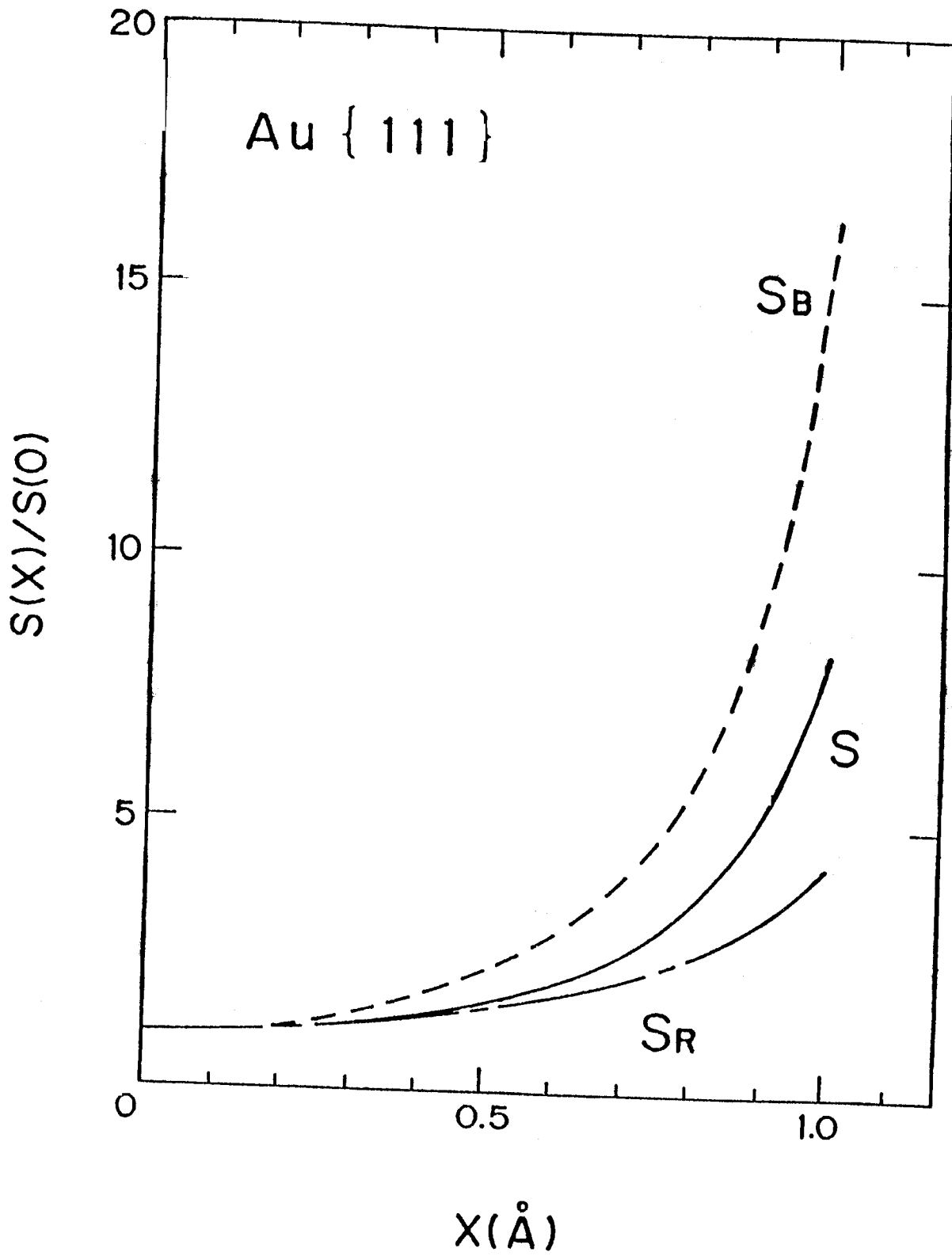


fig.1

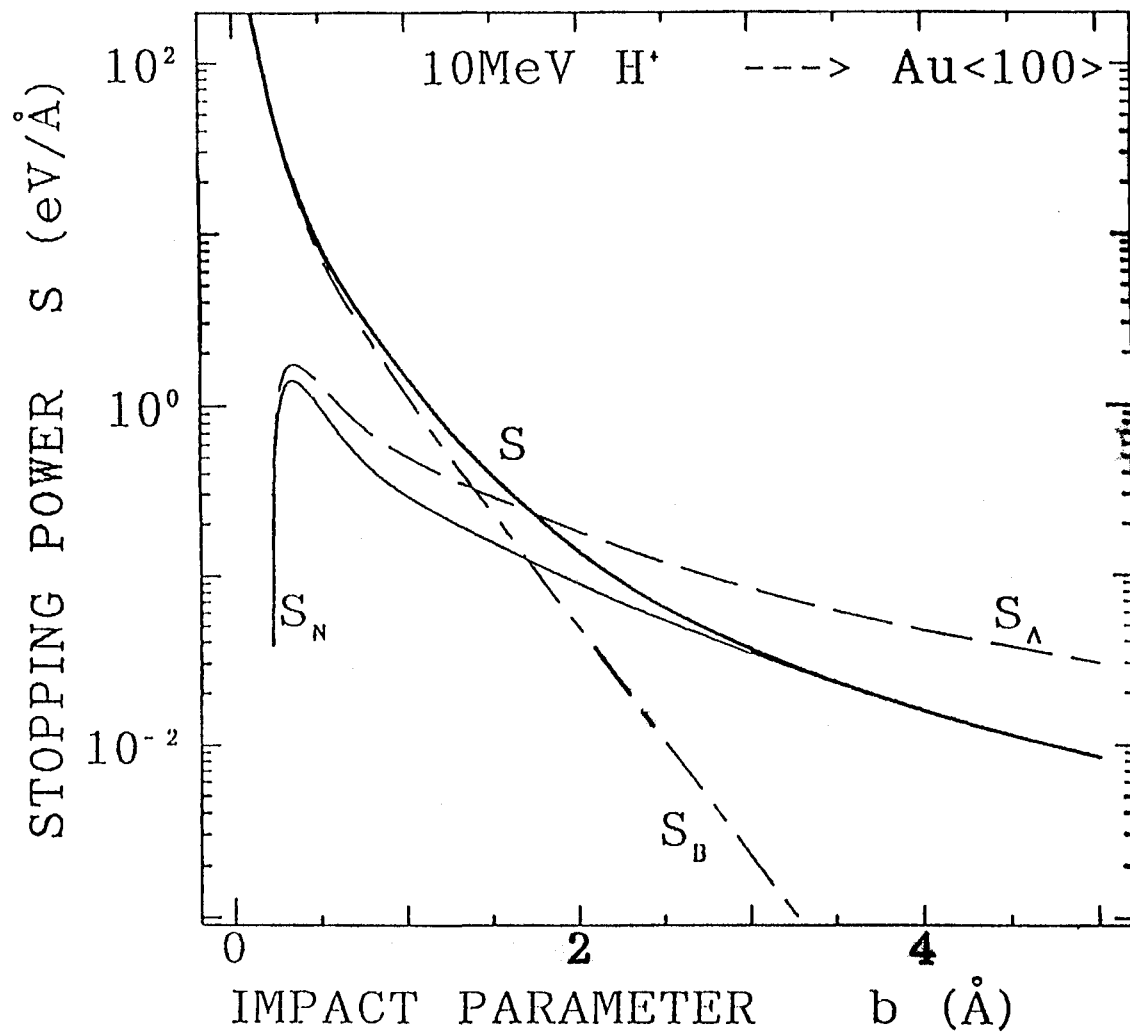


fig.2

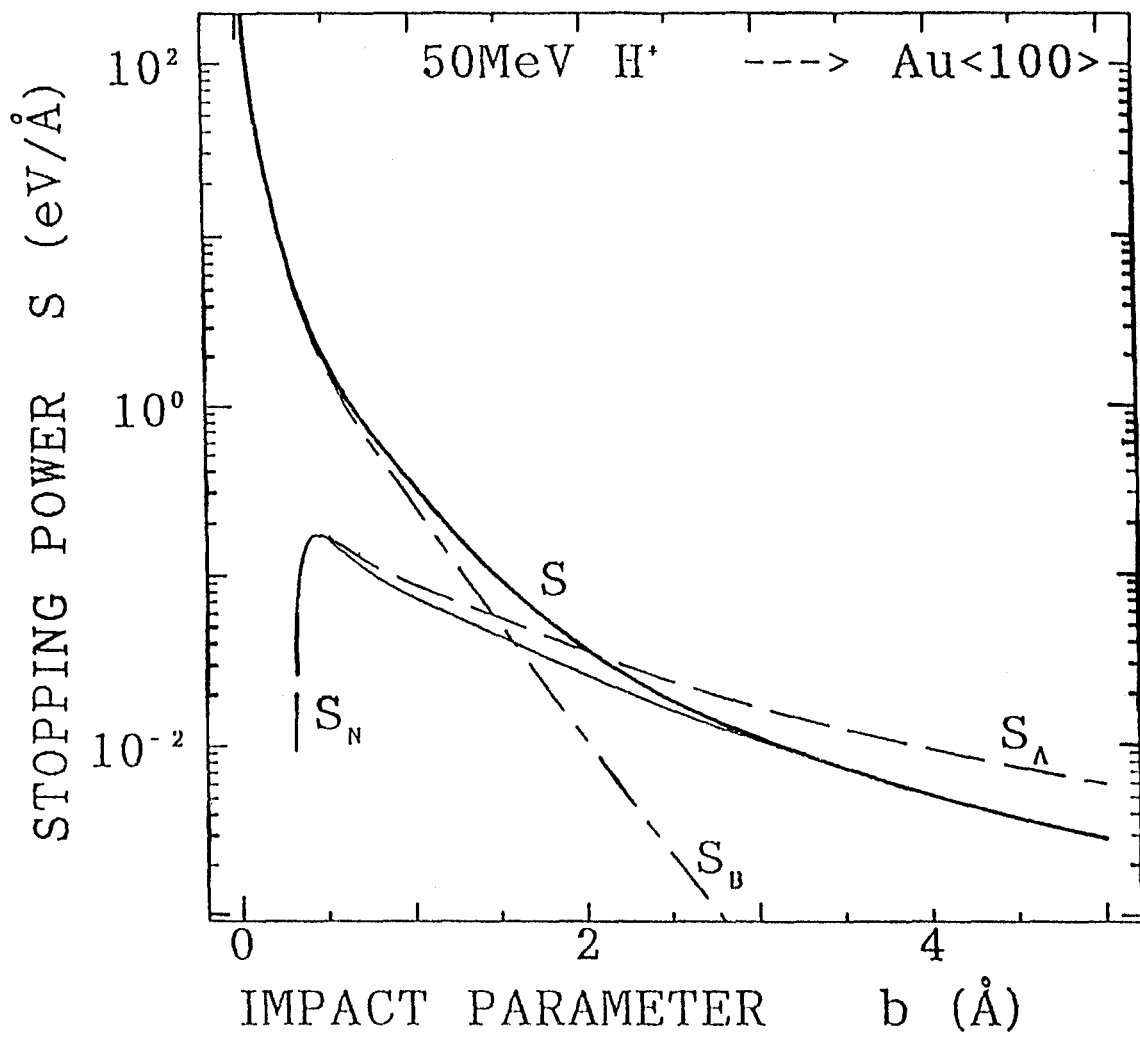


fig.3