Multielectron Dissociative Ionization of Co2 In Intense Laser Fields

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Energy loss of swift metastable projectiles with two bound electrons

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Abstract. An analytical formula for the electronic stopping power S was derived for swift($v \gtrsim Z_1 v_0$) frozen-charge-state projectiles (atomic number Z_1) with two electrons in metastable 1s2s singlet and triplet states, using a first-order perturbation method. The spatial electron distribution around a projectile was determined by the variational method. In order to demonstrate the magnitude of S, we also calculate the effective stopping-power charge. Compared with the ground state ($1s^2$), S in the 1s2s configuration is found to be enhanced especially at the lowest velocity ($v = Z_1 v_0$) investigated. In addition, it is found that (i) there is no appreciable difference between 1s2s singlet and triplet state, and (ii) S for the 1s2s singlet can be scaled in the form $S \times Z_1^{-2.20}$.

1. Introduction

The problem of the energy loss of swift charged particles has been fundamental and essential for scientists working in the fields of atomic collisions in solids and the plasma–first wall interactions. The reason is because this quantity is directly related to the energy deposition of the injected ion beams in a material or the range which they can attain on the average. Also in ion implantation this quantity is applied to analysis of both the depth profile of the implanted atom and the structure of the host lattices in solids.

So far, the electronic stopping power of materials for swift and fully ionized projectiles with velocities v has been investigated intensively. From experimental viewpoints, a lot of measurements have provided valuable data, some of which were recently compiled by Andersen and Ziegler (1977) and Janni (1982). On the other hand, theoretical models and methods have been proposed (Bethe 1930, Bloch 1933, Ritchie 1959, Neufeld and Ritchie 1955, Lindhard and Winther 1964, Sigmund 1982, Echenique *et al* 1986, Gertner *et al* 1978, 1980, Kaneko 1986a, 1989a, b) in order to interpret those data. Recently, theoretical data tables for the stopping power for a proton were also presented on the basis of kinetic theory by Oddershede and Sabin (1984) and wavepacket theory by Kaneko (1993a).

Regarding swift fully-stripped light ions, the energy-loss analyses have been made by means of the Bethe–Bloch theory, if necessary, with including the correction terms. For a point charge $Z_1 e$ moving with velocity v in a material, the electronic stopping

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power S is expressed as (Lindhard 1976)

$$S=(4\pi e^4/mv^2)NZ_2L(Z_1, Z_2, v) \tag{1.1a}$$

$$L(Z_1, Z_2, v)=Z_1^2L_0(Z_2, v)+Z_1^3L_1(Z_2, v)+Z_1^4L_2(Z_2, v). \tag{1.1b}$$

In the above, m, e and N are the electron rest mass, the elementary charge and the number of target atoms of atomic number Z_2 per unit volume, respectively. The leading term $L_0(Z_2, v)$ is given by $L_0(Z_2, v)=\ln(2mv^2/I)$, where I is the mean excitation energy of a material Z_2. The terms $Z_1^3L_1$ and $Z_1^4L_2$ in equation (1.1*b*) are called the Barkas term (Barkas *et al* 1963) and the Bloch correction (Bloch 1933), respectively.

The formula (1.1) cannot be applied to partially stripped ions (PSI). Ferrell and Ritchie (1977) first treated the energy loss of a PSI (i.e. He^+) moving at low velocity in an electron gas. Afterward, the effect of the bound electrons was treated in a statistical model (Brandt and Kitagawa 1982), and in the local electron density models (Kaneko 1986a).

With recent progress in experimental techniques, it has become possible to measure directly the energy loss of a PSI. Cowern *et al* (1984) reported the energy loss of 3 MeV amu^{-1} C^{4-6+} ions in very thin carbon foils. Ogawa *et al* (1991, 1992, 1993) measured the energy-loss of fast hydrogen-like (H-like), helium-like (He-like), and lithium-like (Li-like) ions passing through thin carbon foils with kinetic energy of 10 MeV amu^{-1} under the frozen charge-state condition. To interpret these data theoretically, the analytical stopping-power formulae for H-like and He-like projectiles were derived explicitly (Kaneko 1991) in the form of equation (1.1), but $L(Z_1, Z_2, v)$ must be replaced by

$$L(Z_1, Z_2, v)=(Z_1-N_{1s})^2\ln(2mv^2/I)+(2Z_1N_{1s}-N_{1s}^2)$$
$$\times\ln\{v/(Z_e v_0)\}+Z_1N_{1s}-(11/12)N_{1s}^2. \tag{1.2}$$

Here N_{1s} denotes the number of the 1s electrons so that $Z_e=Z_1$ and $N_{1s}=1$ for H-like and

$$Z_e=Z_1-\tfrac{5}{16} \tag{1.3}$$

and $N_{1s}=2$ for He-like ($1s^2$, singlet) projectiles. The quantity Z_e is related to the screening parameter which will appear in the next section. Moreover for Li-like and Be-like projectiles the stopping-power formulae were also obtained (Kaneko 1993b). In these expressions the Z_1^3 and Z_1^4 terms are neglected.

The above consideration is based on the idea that the ground state configuration may be dominant. The existence of the excited states of projectiles in solids will play a main role in the study of the beam–foil interaction (Andrä 1975, Andrä *et al* 1976). To our regret, there have been no experimental data on the energy loss of excited-state projectiles yet. As a basic knowledge, however, theoretical prediction of this quantity will become important. Therefore, as a first step, we present here an analytical formula for the electronic energy loss of swift metastable projectiles in electron configuration 1s2s for the first time. Both a singlet and a triplet state are considered here. First, section 2 is devoted to a description of the theoretical procedure. Results and discussion are given in section 3. Throughout this paper, m, e, a_0, v_0 and $\hbar$ denote the electron rest mass, the elementary charge, the Bohr radius ($=0.529\times10^{-8}$ cm), the Bohr velocity ($=2.19\times10^8$ cm s^{-1}) and the Planck constant divided by 2π, respectively.

2. Theory

Here we assume that the projectile velocity v is larger than both the average velocity of the target electrons, $Z_2^{2/3}v_0$, and that of the projectile electron, $Z_e v_0$. Hence we can use the first Born approximation. Second, the electronic state of the projectile is completely frozen during the passage of the projectile. This assumption (a 'frozen charge state') is actually valid if a fast projectile penetrates a very thin foil.

We now discuss the validity of the frozen-charge-state condition. The condition of $v > Z_e v_0$ means that the electron loss process is much more dominant than the electron capture process, as the velocity-stripping criterion suggests (Bohr 1948). In this velocity region, the survival fraction ϕ of particles penetrating to depth z with a charge equal to the incident decreases like $\exp(-z/\lambda)$, where λ denotes the attenuation length. As the penetration depth increases, the value of ϕ will deviate from a simple exponential function and finally it reaches the equilibrium fraction ϕ_{eq}, dependent upon the velocity (Gaillard *et al* 1977). Since the capture cross section can be negligibly small (i.e. ϕ_{eq} is very small), λ is approximately given by $1/(\sigma_{loss}N)$, where σ_{loss} is the one-electron loss cross section for the incident particle, and N the number of target atoms per unit volume. Therefore, the pre-equilibrium charge-state depth z_{pre} is approximately characterized by

$$z_{pre} = \ln(1/\phi_{eq})/(\sigma_{loss}N). \tag{2.1}$$

Of course this value depends on the projectile velocity via ϕ_{eq} and σ_{loss}. The electron-loss cross section is inversely proportional to the binding energy (Rule 1977, Kaneko 1986b). Then based on a hydrogen-like model, the loss cross section $\sigma_{loss,n}$ for an excited state with principal quantum number n is approximately represented by $n^2\sigma_{loss,1s}$. Hence the concept of the frozen charge state has meaning only in a thin foil region of $z < (1/n^2)z_{pre,1s}$, where $z_{pre,1s}$ is the pre-equilibrium depth for the 1s state.

2.1. Distribution of the projectile electrons

Here we determine the spatial distribution of two electrons bound on the projectile. Here one electron is assigned to the 1s and the other electron to the 2s state. In order to satisfy the Pauli principle, the wavefunction of this two-electron system has to be antisymmetric with respect to mutual exchange of electrons. Symmetry in space correlates with antisymmetry in spin. Now the spin–orbital interaction is neglected so that the one-electron state can be described by the product of the wavefunction in space and that in spin.

Let us define the spin wavefunctions for the up-spin and the down-spin state, respectively, by $\alpha(\sigma)$ and $\beta(\sigma)$, where σ is spin variable. As well, the wavefunctions in space for the 1s and 2s states are denoted by $\psi_{1s}(r)$ and $\psi_{2s}(r)$. Then, the total wavefunction Ψ_S for the singlet spin state is expressed in terms of

$$\Psi_S = \psi_S(r_1, r_2)\chi_S(\sigma_1, \sigma_2) \tag{2.2a}$$

where

$$\psi_S(r_1, r_2) = (2)^{-1/2}[\psi_{1s}(r_1)\psi_{2s}(r_2) + \psi_{1s}(r_2)\psi_{2s}(r_1)] \tag{2.2b}$$

$$\chi_S(\sigma_1, \sigma_2) = (2)^{-1/2}[\alpha(\sigma_1)\beta(\sigma_2) - \alpha(\sigma_2)\beta(\sigma_1)]. \tag{2.2c}$$

Similarly, the wavefunction Ψ_T for the triplet spin state is expressed as

$$\Psi_T = \psi_T(r_1, r_2)\chi_T(\sigma_1, \sigma_2) \tag{2.3a}$$

where

$$\psi_T(r_1, r_2) = (2)^{-1/2}[\psi_{1s}(r_1)\psi_{2s}(r_2) - \psi_{1s}(r_2)\psi_{2s}(r_1)] \tag{2.3b}$$

and

$$\chi_T(\sigma_1, \sigma_2) = \begin{cases} \alpha(\sigma_1)\alpha(\sigma_2) \\ (2)^{-1/2}[\alpha(\sigma_1)\beta(\sigma_2) + \alpha(\sigma_2)\beta(\sigma_1)] \\ \beta(\sigma_1)\beta(\sigma_2). \end{cases} \tag{2.3c}$$

The spatial wavefunctions $\psi_{1s}(r)$ and $\psi_{2s}(r)$ are assumed to have the following forms:

$$\psi_{1s}(r) = (\pi a^3)^{-1/2} \exp(-r/a) \tag{2.4a}$$

$$\psi_{2s}(r) = (4\pi)^{-1/2}(2a)^{-3/2}(2 - r/a) \exp(-r/2a). \tag{2.4b}$$

It is obvious that these normalized functions are orthogonal to each other. In equation (2.4), a is the orbital screening parameter, depending on the nuclear charge Z_1 of the projectile. In order to determine it, we minimize the total energy, which was calculated both for the singlet and triplet states in quantum-mechanical manner. Let us consider the Hamiltonian of the system composed of 1s and 2s electrons.

$$H = \sum_{i=1,2} H_i + V_{12} \tag{2.5a}$$

$$H_i = (-\hbar^2/2m)\Delta_i - Z_1 e^2/r_i \tag{2.5b}$$

$$V_{12} = e^2/|r_1 - r_2|. \tag{2.5c}$$

Using equations (2.5), the expectation value of H for the singlet, $\langle H \rangle_S$, is calculated as follows

$$\langle H \rangle_S = E_{1s} + E_{2s} + V_{1s\text{-}2s} + K_{1s\text{-}2s} \tag{2.6a}$$

$$E_{1s} = \hbar^2/(2ma^2) - Z_1 e^2/a \tag{2.6b}$$

$$E_{2s} = \tfrac{1}{4} E_{1s} \tag{2.6c}$$

$$V_{1s\text{-}2s} = e^2 \int dr \int dr' \, |\psi_{2s}(r)|^2 |\psi_{1s}(r')|^2 / |r - r'|$$

$$= 17e^2/81a \tag{2.6d}$$

$$K_{1s\text{-}2s} = \int dr \int dr' \, \psi_{1s}(r)^* \psi_{2s}(r')^* (e^2/|r - r'|) \psi_{1s}(r') \psi_{2s}(r)$$

$$= 16e^2/729a. \tag{2.6e}$$

In the above equations, $V_{1s\text{-}2s}$ and $K_{1s\text{-}2s}$ are, respectively, the direct Coulomb integral and the exchange integral. For the triplet state, on the other hand, the sign of the

exchange integral is negative so that the total energy $\langle H\rangle_T$ has the following form:

$$\langle H\rangle_T = E_{1s} + E_{2s} + V_{1s\text{-}2s} - K_{1s\text{-}2s} \tag{2.7}$$

where all notations are the same as in equation (2.6).

For convenience, a new parameter Z_e is introduced instead of a by $a = a_0/Z_e$. Then, one obtains in units of e^2/a_0

$$\langle H\rangle_S = \tfrac{5}{8}\{Z_e - (Z_1 - \tfrac{676}{3645})\}^2 - \tfrac{5}{8}(Z_1 - \tfrac{676}{3645})^2 \tag{2.8}$$

$$\langle H\rangle_T = \tfrac{5}{8}\{Z_e - \{Z_1 - \tfrac{548}{3645})\}^2 - \tfrac{5}{8}(Z_1 - \tfrac{548}{3645})^2. \tag{2.9}$$

As one can easily see, these are parabolic functions with respect to Z_e so that they take a minimum at $Z_e = Z_1 - \frac{676}{3645}$ and at $Z_e = Z_1 - \frac{548}{3645}$. Thus the orbital parameter a, or Z_e, can be determined by the energy-minimizing variational method. The variable Z_e is interpreted as the screened *nuclear charge* for the 1s2s configuration system. If there is only one bound electron, this system reduces to a hydrogenic one, resulting in $Z_e = Z_1$. In our treatment, therefore, a two-electron system on a projectile is governed by the hydrogen-like orthonormal orbitals defined under the screened nuclear charges of the forms

$$Z_e(1s\text{–}2s, \text{singlet}) = Z_1 - \tfrac{676}{3645} \tag{2.10a}$$

$$Z_e(1s\text{–}2s, \text{triplet}) = Z_1 - \tfrac{548}{3645}. \tag{2.10b}$$

It is worthwhile comparing equations (2.9) to the corresponding quantity (1.3) for the $1s^2$ ground state (singlet). From equations (2.10) and (1.3), the degree of screening in the $1s^2$ state is stronger than in the metastable 1s2s state by 0.13–0.16.

2.2. *Stopping-power formula*

As usual, let us begin with a general expression of the electronic stopping power S in the Born approximation as follows (Kim and Cheng 1980, Gillespie and Inokuti 1980):

$$S = N\sum_n (E_n - E_0)\int_{q_{min}}^{q_{max}} (dq/q^3)8\pi(e^2/\hbar v)^2 |F_{00}^p(-q)|^2 |F_{n0}^t(q)|^2. \tag{2.11}$$

In the above, E_n and E_0 denote the eigenenergies of the target-material states n and 0, respectively. N is the number of target atoms per unit volume. The momentum transferred to the target electrons ranges from $\hbar q_{min} = (E_n - E_0)/v$ to $\hbar q_{max} = 2mv$. The form factor of the projectile, $F_{00}^p(-q)$, and inelastic scattering amplitude of the target atom, $F_{n0}^t(q)$, are given by

$$F_{00}^p(-q) = Z_1 - \langle 0|\sum_i \exp(+iqr_i)|0\rangle \tag{2.12}$$

$$F_{n0}^t(q) = \langle n|\sum_j \exp(-iqr_j)|0\rangle. \tag{2.13}$$

The function $F_{00}^p(-q)$ is calculated by the Fourier transform of the spatial distribution of the configuration for the 1s2s singlet and the 1s2s triplet. As $\langle 0|\sum_i \exp(iqr_i)|0\rangle$ is denoted by $\rho(q)$, we have

$$\rho(q) = \rho_{1s}(q) + \rho_{2s}(q) \tag{2.14a}$$

$$\rho_{1s}(q) = [1 + (\tfrac{1}{2}qa)^2]^{-2}, \tag{2.14b}$$

$$\rho_{2s}(q) = [2(qa)^2 - 1][(qa)^2 - 1]/[1 + (qa)^2]^4. \tag{2.14c}$$

It is convenient to divide the integration region $[q_{\min}, q_{\max}]$ into two sections, i.e. $A=[q_{\min}, q_0]$ and $B=[q_0, q_{\max}]$, where q_0 is such an appropriate parameter that the dipole approximation can be applied to $F^{t}_{n0}(q)$. Hereby we have $\exp(-\mathrm{i}\boldsymbol{q}\boldsymbol{r}_j)=1-\mathrm{i}\boldsymbol{q}\boldsymbol{r}_j$ and the contribution from section A, S_A, is then reduced to

$$S_A = N\sum_n (E_n - E_0)8\pi(e^2/\hbar v)^2 |\boldsymbol{d}_{n0}|^2 \int_{q_{\min}}^{q_0} (\mathrm{d}q/q)|F^{B}_{00}(-\boldsymbol{q})^2 \tag{2.15}$$

where $\boldsymbol{d}_{n0}$ is the dipole matrix element. On the other hand, the contribution from section B, S_B, is expressed as

$$S_B = N(\hbar^2/2m)Z_2 8\pi(e^2/\hbar v)^2 \int_{q_0}^{q_{\max}} (\mathrm{d}q/q)|F^{B}_{00}(-\boldsymbol{q})|^2. \tag{2.16}$$

Here one can interchange the order of the summation over n and the integration over q since both $q_{\max}$ and q_0 are independent of the eigenstate $|n\rangle$. Thus we are able to employ the sum rule (Landau and Lifshitz 1958)

$$\sum_n (E_n - E_0)|F^{t}_{n0}(\boldsymbol{q})|^2 = (\hbar^2 q^2/2m)Z_2. \tag{2.17}$$

Fortunately, the definite integrals in S_A and S_B are straightforwardly estimated if one uses the following analytical result of the indefinite integral:

$$2\int (\mathrm{d}q/q)|F^{B}_{00}(-\boldsymbol{q})|^2$$

$$= A\ln(q^2a^2) + f(q^2a^2+1) + g(q^2a^2+4) + \text{integral constant}. \tag{2.18}$$

Here the functions $f(x)$ and $g(x)$ are defined by

$$f(x) = B_0\ln(x) + \sum_{j=1}^{7} B_j/x^j \tag{2.19}$$

$$g(x) = C_0\ln(x) + \sum_{j=1}^{3} C_j/x^j. \tag{2.20}$$

In equations (2.18)–(2.20), A, B_i ($i=1$–7) and C_i ($i=1$–3) are the following constants:

$$\begin{aligned}
&A=(Z_1-2)^2 \qquad B_0=2Z_1+\tfrac{175}{81} \qquad B_1=\tfrac{379}{27}-2Z_1 \qquad B_2=Z_1-\tfrac{151}{18}\\
&B_3=\tfrac{67}{9}-4Z_1 \qquad B_4=-\tfrac{3}{4} \qquad B_5=5 \qquad B_6=-8 \qquad B_7=\tfrac{36}{7}\\
&C_0=2Z_1-\tfrac{499}{81} \qquad C_1=\tfrac{76}{9}-8Z_1 \qquad C_2=8 \qquad C_3=\tfrac{64}{3}.
\end{aligned} \tag{2.21}$$

At this point, we remember that the high but non-relativistic velocity case is now considered. Therefore, we can naturally assume that $a^2q^2_{\min}\ll 1$, namely, $(E_n-E_0)/(\hbar v/a_0)\ll Z$(1s–2s, singlet) (or Z(1s–2s, triplet)) and $a^2q^2_{\max}\gg 4$, namely, $v/v_0\gg Z$(1s–2s, singlet) (or Z(1s–2s, triplet)) hold valid in this energy region. Then, using the sum rule (Landau and Lifshitz 1958)

$$\sum_n (E_n - E_0)|\boldsymbol{d}_{n0}|^2 = (\hbar^2/2m)Z_2 \tag{2.22}$$

and the approximations

$$f(a^2q_{\min}^2+1)=\sum_{i=1}^{7}B_i+\left\{B_0-\sum_{i=1}^{7}iB_i\right\}(q_{\min}a)^2+O(q_{\min}^4a^4) \tag{2.23}$$

$$g(a^2q_{\min}^2+4)=C_0\ln 4+\sum_{i=1}^{3}C_i/4^i+\left\{C_0/4-\sum_{i=1}^{3}iC_i/4^{(i+1)}\right\}(q_{\min}a)^2+O(q_{\min}^4a^4) \tag{2.24}$$

we get

$$S_A=(2\pi e^4/mv^2)NZ_2\Bigg[2A\ln(q_0a)+f(q_0^2a^2+1)+g(q_0^2a^2+4)-2A\ln(Ia/hv)$$
$$-\sum_{i=1}^{7}B_i-C_0\ln 4-\sum_{i=1}^{3}C_i/4^i-\left\{B_0\sum_{i=1}^{7}iB_i+\tfrac{1}{4}C_0-\sum_{i=1}^{3}iC_i/4^{(i+1)}\right\}$$
$$\times(2m/\hbar^2Z_2)G_3(a/\hbar v)^2-O(G_5(a/\hbar v)^4)\Bigg]. \tag{2.25}$$

Here I denotes the mean excitation energy, defined by

$$\ln I=(1/Z_2)(2m/\hbar^2)\sum_n(E_n-E_0)|d_{n0}|^2\ln(E_n-E_0) \tag{2.26}$$

and

$$G_m=\sum_n(E_n-E_0)^m|d_{n0}|^2 \qquad (m=3,5). \tag{2.27}$$

In this equation, G_m denotes the mth excitation energy moment of the dipole transition probability. The first moment G_1 leads to the well known sum rule (2.22).

Similarly, using the approximations

$$f(a^2q_{\max}^2+1)=B_0\ln(a^2q_{\max}^2)+(B_0+B_1)(q_{\max}a)^{-2}+O((q_{\max}a)^{-4}) \tag{2.28}$$

and

$$g(a^2q_{\max}^2+4)=C_0\ln(a^2q_{\max}^2)+(4C_0+C_1)(q_{\max}a)^{-2}+O((q_{\max}a)^{-4}) \tag{2.29}$$

we have

$$S_B=(2\pi e^4/mv^2)NZ_2[2(A+B_0+C_0)\ln(2mva/\hbar)-2A\ln(q_0a)-f(q_0^2a^2+1)$$
$$-g(q_0^2a^2+4)+(B_0+B_1+4C_0+C_1)(\hbar^2/2m^2v^2a^2)$$
$$+O((2mva/\hbar)^{-4}]. \tag{2.30}$$

Summing S_A in equation (2.25) and S_B in equation (2.30), the total electronic stopping power S for singlet and triplet states can be represented in the form

$$S=(4\pi e^4/mv^2)NZ_2L \tag{2.31a}$$

where

$$L=(Z_1-2)^2\ln(2mv^2/I)+4(Z_1-1)\ln(v/Z_ev_0)+(2Z_1+\tfrac{175}{81})\ln(2)+\tfrac{7}{2}Z_1-\tfrac{13177}{1512} \tag{2.31b}$$

where $Z_e = Z(1s\text{-}2s, \text{singlet})$ for the singlet state and $Z_e = Z(1s\text{-}2s, \text{triplet})$ for the triplet state. We remark here that in the above equation, the character of a target atom is represented by the only one parameter I. Note that q_0 cancel out in the total stopping power S. The leading correction term to equation (2.31*b*) is of the order of v^{-2}, representing

$$\Delta L = -15(Z_1 - 2)(2mG_3/\hbar^2 Z_2)/(mv_0 v Z_e)^2. \tag{2.32}$$

Hereafter we only focus on the leading term L, because the correction ΔL can be omitted together with other higher-order terms in the velocity region considered.

As an application of (2.31), we present here the stopping power for swift neutral projectiles. By setting $Z_1 = 2$, one gets the quantity L (equations (2.31*b*) and (1.2)) for a metastable helium atom as

$$L_{\text{meta-He}} = 4\ln(v/Z_e v_0) + \tfrac{499}{81}\ln(2) - \tfrac{2593}{1512} \tag{2.33a}$$

where Z_e is given by (2.10). On the other hand, from (1.2) and (1.3), for the ground state ($1s^2$, singlet) helium atoms, L reduces to

$$L_{\text{He}} = 4\ln(16v/27v_0) + \tfrac{1}{3}. \tag{2.33b}$$

It is noted that the characteristic parameter I of a target does not appear in the above equations. In other words, the energy loss depends not on the microscopic quantum states of the target but on the macroscopic target parameters, i.e. N and Z_2, as well as on the projectile parameters. Hence, the stopping cross section for these atoms *in the charge-state pre-equilibrium region* is completely proportional to the target atomic number Z_2. This is because the projectile excitation process is not taken into account.

2.3. The effective stopping-power charge

In order to comprehend and compile the stopping power data for partially stripped ions, the concept of the effective charge Z_{eff} is useful. This idea is based on the Bethe formula (equation (1.1*a*) with $L = Z_1^2 \ln(2mv^2/I)$) for a point charge intruder. According to this formula, the quantities characterizing a projectile are the charge $Z_1 e$ and the velocity v so that S is proportional to Z_1^2 at constant velocity. Then in order to conjecture the magnitude of the stopping power, it is convenient to define the effective stopping-power charge in the frozen charge state, $Z_{\text{eff}}^{\text{f}}$, as

$$Z_{\text{eff}}^{\text{f}} = (S/S_{\text{p}})^{1/2} \tag{2.34}$$

where S_{p} is the stopping power for a proton ($Z_1 = 1$) at the same velocity as the projectile considered. At this point, the effective charge means the magnitude of electric charge of a projectile seen through the stopping power. The $Z_{\text{eff}}^{\text{f}}$ is different from the conventional effective charge Z_{eff}. There are two effects on the Z_{eff}. One is the charge-changing effect inside a target and the other is the size effect of a projectile. The former is due to the fact that at least several charge-state components have contributed to the stopping power S. In recent frozen-charge-state measurements, however, the first effect cannot appear. In this sense, the $Z_{\text{eff}}^{\text{f}}$ obtained here reflects the size effect only. In general, the $Z_{\text{eff}}^{\text{f}}$ and Z_{eff} for ion species A^{q+} are different from the net charge qe. Moreover, Z_{eff} is dependent on but not equal to the average charge q_{mean}. Actually, due to close collisions, $Z_{\text{eff}}(Z_{\text{eff}}^{\text{f}})$ is rather greater than q_{mean} (q) especially for low-velocity ion-beams (frozen-charge-state ions) (e.g. Kaneko 1984, 1986a).

According to the definition, the $Z_{\rm eff}^{\rm f}$ for the projectile in a metastable 1s2s configuration is found to be

$$Z_{\rm eff}^{\rm f}=[(Z_1-2)^2+[\ln(2mv^2/I)]^{-1}\{4(Z_1-1)\ln(v/Z_{\rm e}v_0)+(2Z_1+\tfrac{175}{81})\ln(2)+\tfrac{7}{2}Z_1-\tfrac{13177}{1512}\}]^{1/2}. \tag{2.35}$$

One should keep in mind that the above expression is not for fast ions undergoing electron stripping or exchange collisions but for ions of the same charge-state as the incident one. Therefore, the formula (2.35) is different from the $Z_{\rm eff}$, which monotonically goes to Z_1 with increasing ion velocity. This is due to the charge-changing effect. Namely, the fact that the bound electrons will be stripped off more and more as the velocity increases, plays a key role. However, this is not our case. Here, even at high velocities, the bound electrons are assumed to still attach to the ion moving in a very thin foil. In the limit of extremely high velocity, i.e. $v\gg Z_{\rm e}v_0$ and $v\gg(I/2m)^{1/2}$, equation (2.35) becomes saturated at the value

$$Z_{\rm eff}^{\rm f}=(Z_1^2-2Z_1+2)^{1/2} \tag{2.36}$$

which is independent of the ion velocity. It is noted here that the above value is determined only by the number of bound electrons. As is expected, the ground state $1s^2$ configuration also yields the same $Z_{\rm eff}^{\rm f}$ value.

In order to see a systematic feature, let us have the following expression of $Z_{\rm eff}$ for hydrogen-like and helium-like ($1s^2$) projectiles (Kaneko 1991):

$$Z_{\rm eff}^{\rm f}=[(Z_1-N_{1s})^2+[\ln(2mv^2/I)]^{-1}N_{1s}\{(2Z_1-N_{1s})\ln(v/Z_{\rm e}v_0)+Z_1-\tfrac{12}{11}N_{1s}\}]^{1/2} \tag{2.37}$$

where N_{1s} denotes the number of 1s electrons. One has, for hydrogen-like projectiles, $Z_{\rm e}=Z_1$ and $N_{1s}=1$, and on the other hand, for helium-like ones, $Z_{\rm e}=Z_1-\frac{5}{16}$ and $N_{1s}=2$. At high velocities (2.37) reduces to

$$Z_{\rm eff}^{\rm f}=[(Z_1-N_{1s})^2+Z_1N_{1s}-\tfrac{1}{2}N_{1s}^2]^{1/2}. \tag{2.38}$$

This result is also independent of velocity. By setting $N_{1s}=2$ one sees that equation (2.38) gets the same value as equation (2.36).

3. Numerical results and discussion

Figure 1 shows the stopping cross section $S(1s^2)/N$ of carbon calculated from (1.2) with $I=77.3$ eV $=2.842$ au (Andersen *et al* 1977) for helium-like ground-state ($1s^2$) projectiles with atomic number $Z_1=2$, 4, 6 and 8 and with velocity from $v=Z_1v_0$ to $v=60v_0$. Figure 2 displays the stopping cross section, S(1s2s, singlet), of carbon calculated from (2.31) for the corresponding projectiles in the metastable 1s2s singlet state. In order to estimate the difference between in the $1s^2$ and in the 1s2s state, we plot in figure 3 the ratio of S(1s2s, singlet)/$S(1s^2)$. At velocities $v\gtrsim Z_1v_0$ it becomes greater than 2 for small Z_1, while with increasing velocity it gradually decreases, approaching unity. Such an enhancement in the metastable stopping is not so large for the larger Z_1 values. This result can be explained as follows. In general, as the Z_1 value increases, the average radius of the bound electron becomes shorter since, roughly speaking, the radius is inversely proportional to Z_1. Then the screening of the ion nuclear charge by the bound electrons is more complete and thereby the net-charge approximation becomes valid for heavier (or larger Z_1) ions. In other words, formula (2.31*b*) is apt to be dominantly

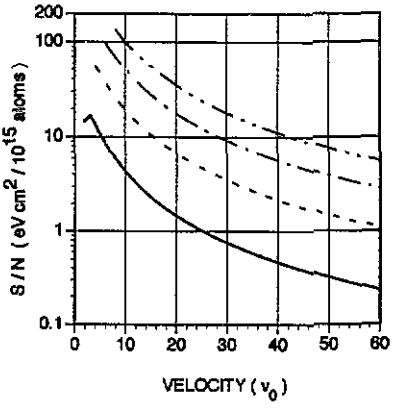

Figure 1. The calculated stopping cross section, $S(1s^2)/N$, of carbon ($I=77.3$ eV) as a function of velocity v for helium-like ground-state ($1s^2$) projectiles with $Z_1=2$ (——), $Z_1=4$ (- - -), $Z_1=6$ (— - —) and $Z_1=8$ (— - - —).

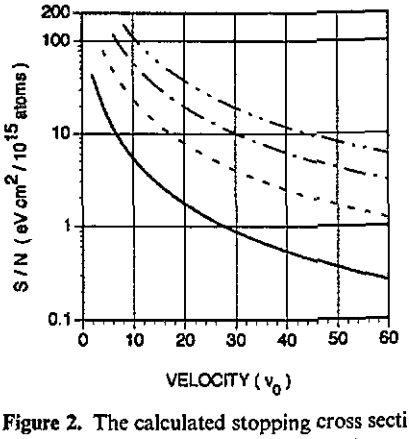

Figure 2. The calculated stopping cross section, $S(1s2s, \text{singlet})/N$, of carbon as a function of velocity v for helium-like metastable-state (1s2s, singlet) projectiles with $Z_1=2$ (——), $Z_1=4$ (- - -), $Z_1=6$ (— - —) and $Z_1=8$ (— - - —).

governed by the first term so that the ion can be regarded as a point charge. This picture leads to another conclusion that the effective stopping-power charge Z^f_{eff} reduces asymptotically to the net charge.

Regarding the 1s2s triplet projectiles, no appreciable difference is found in the stopping between the 1s2s singlet and the 1s2s triplet state. To see in detail, however, the relative difference, $[S(1s2s, \text{singlet}) - S(1s2s, \text{triplet})]/S(1s2s, \text{triplet}) \times 100$ is shown in figure 4. One can see that this value is within 3% over the whole velocity range considered, and that this becomes smaller with increasing velocity.

As stated above, it is convenient to convert the electronic stopping power into the effective charge Z^f_{eff}. Figure 5 shows the Z^f_{eff} of swift C^{4+} and O^{6+} ions both in the ground state ($1s^2$) and the 1s2s singlet state. It is found that in going from the ground state to the excited state Z^f_{eff} increases by 0.5 at low velocities and by 0.2 at high velocities.

Finally figure 6 indicates that scaling of the electronic stopping cross sections can be possible for the helium-like metastable (1s2s) projectiles with $Z_1>3$. The scaling

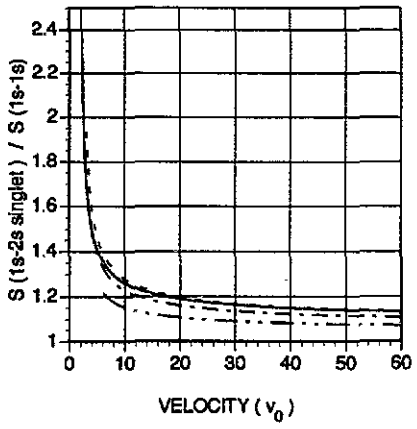

Figure 3. The ratio of $S(1s2s, \text{singlet})$ to $S(1s^2)$ for $Z_1=2$ (——), $Z_1=3$ (- - -), $Z_1=4$ (— - —) and $Z_1=6$ (— - - —) as a function of velocity.

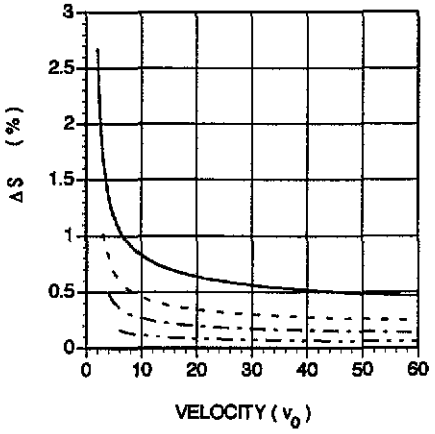

Figure 4. The ratio, $\Delta S=[S(1s2s, \text{singlet})-S(1s2s, \text{triplet})]/S(1s2s, \text{triplet})$, expressed in per cent, as a function of velocity for $Z_1=2$ (——), $Z_1=3$ (- - -), $Z_1=4$ (— - —) and $Z_1=6$ (— - - —).

factor $Z_1^{-2.20}$ is numerically found by the least-squares fitting of the calculated stopping values for $Z_1=3, 4, 6, 8, 10, 20$ and 30 at $v=30v_0$. In the figure we draw the scaled stopping curves $S\times Z_1^{-2.20}$ for $Z_1=3, 4, 6, 8, 10, 20$ and 30 in the velocity range $Z_1v_0\leqslant v\leqslant 100v_0$. In spite of fitting at a particular velocity, the obtained curve is well scaled over the whole range of velocity. At $v=60v_0$ the power of Z_1 in the scaling factor is -2.205 which is very near to the case of $v=30v_0$. This scaling factor is almost constant at high velocities. At lower velocities, e.g. $v=10v_0$, and $20v_0$, the power becomes -2.218, deviating a bit from -2.20. This means that the six scaled curves do not look like one universal curve in the low velocity region.

In conclusion, the analytical expression for the electronic stopping power for the metastable 1s2s helium-like projectiles in a frozen charge state was presented on the basis of the first-order perturbation theory and the Hartree–Fock–Slater method. The leading correction term $\Delta L(Z_1, Z_2, v)$ at high velocity was also presented. Enhancement

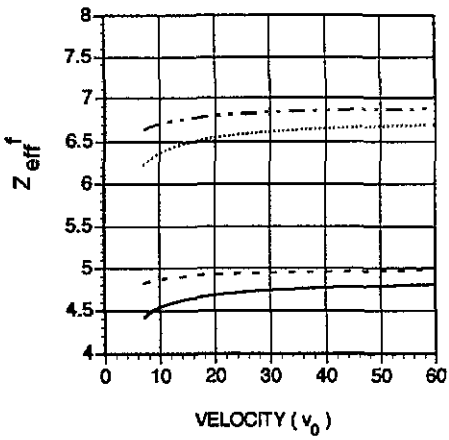

Figure 5. The effective charge, Z_{eff}^{f}, of $C^{4+}(Z_1=6)$ and $O^{6+}(Z_1=8)$ ions in the $1s^2$ state (——, $Z_1=6$; - - - - - - -, $Z_1=8$) and 1s2s singlet (– – –, $Z_1=6$; — — —, $Z_1=8$) in carbon.

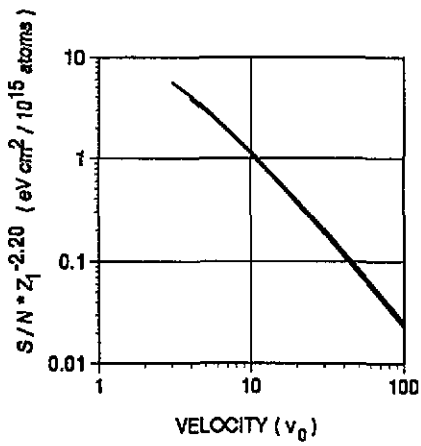

Figure 6. The scaled stopping cross section, $S(1s2s, \text{singlet})/N \times Z_1^{-2.20}$ for swift projectiles in the 1s2s singlet state in carbon.

in the stopping power for the metastable projectiles occurs, especially at the lowest velocity $v = Z_1 v_0$, and consequently, the effective stopping-power charge of those projectiles becomes larger than that of the ground-state ($1s^2$) projectile. No appreciable difference in the electronic stopping is found between the 1s2s singlet and the 1s2s triplet state. A scaling law could also be found numerically for the 1s2s electronic stopping curve. To our regret, there are no experimental data on the projectiles in excited states as far as the authors know. We think, however, these results will be useful to analyse energy-loss data in which excited states are incorporated. Investigation of the energy-loss of swift ions with a 2p electron is now in progress and will be published in the near future.

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References

Andersen H H and Ziegler J F 1977 *The Stopping and Ranges of Ions in Matter* (New York: Pergamon)
Andrä H J 1975 *Phys. Lett.* **54A** 315
Andrä H J, Frohling R, Plohn H J and Silver J D 1976 *Phys. Rev. Lett.* **37** 1212
Barkas W H, Dyer N J and Heckman H H 1963 *Phys. Rev. Lett.* **11** 26
Bethe H A 1930 *Ann. Phys. Lpz.* **5** 325
Bloch F 1933 *Ann. Phys. Lpz.* **16** 285
Bohr N 1948 *K. Dansk. Vidensk. Selsk. Mat.-Fys. Meddr.* **18** 8
Brandt W and Kitagawa M 1982 *Phys. Rev.* B **25** 5631
Cowern N E B, Read P M, Sofield C J, Bridwell L B and Lucas M W 1984 *Phys. Rev.* A **30** 1682
Echenique P M, Nieminen R M, Ashley J C and Ritchie R H 1986 *Phys. Rev.* A **33** 897
Ferrell T L and Ritchie R H 1977 *Phys. Rev.* B **16** 115
Gaillard M J, Poizat J C, Ratkowski A, Remillieux J and Auzas M 1977 *Phys. Rev.* A **16** 2323
Gertner I, Meron M and Rosner B 1978 *Phys. Rev.* A **18** 2022
—— 1980 *Phys. Rev.* A **21** 1191
Gillespie G H and Inokuti M 1980 *Phys. Rev.* A **22** 2430
Janni J F 1982 *At. Data Nucl. Data Tables* **27** 147
Kaneko T 1984 *Phys. Rev.* A **30** 1714
—— 1986a *Phys. Rev.* A **33** 1602
—— 1986b *Phys. Rev.* A **34** 1779
—— 1989a *Phys. Rev.* A **40** 2188
—— 1989b *Phys. Stat. Sol.* B **156** 49
—— 1991 *Phys. Rev.* A **43** 4780
—— 1993a *At. Data Nucl. Data Tables* **53** 271
—— 1993b submitted
Kim Y-K and Cheng K-T 1980 *Phys. Rev.* A **22** 61
Landau L D and Lifshitz E M 1958 *Quantum Mechanics* (London: Pergamon)
Lindhard J 1976 *Nucl. Instrum. Methods* **132** 1
Lindhard J and Winther A 1964 *K. Dansk. Vidensk. Selsk. Mat.-Fys. Meddr.* **34** (4) 1
Neufeld J and Ritchie R H 1955 *Phys. Rev.* **98** 1632
Oddershede J and Sabin J R 1984 *At. Data Nucl. Data Tables* **31** 275
Ogawa H, Katayama I, Ikegami H, Haruyama Y, Aoiki A, Tosaki M, Fukuzawa F, Yoshida K, Sugai I and Kaneko T 1991 *Phys. Rev.* B **43** 11370
Ogawa H, Katayama I, Sugai I, Haruyama Y, Saito M, Yoshida K, Tosaki M and Ikegami H 1993 *Nucl. Instrum. Methods* B **82** 80
Ogawa H, Katayama I, Sugai I, Haruyama Y, Tosaki M, Aoki A, Yoshida K and Ikegami H 1992 *Phys. Lett.* **167A** 487
Ritchie R H 1959 *Phys. Rev.* **114** 644
Rule D W 1977 *Phys. Rev.* A **16** 19
Sigmund P 1982 *Phys. Rev.* A **26** 2497