Nuclear Instruments and Methods in Physics Research B 315 (2013) 76–80

Contents lists available at SciVerse ScienceDirect

Nuclear Instruments and Methods in Physics Research B

journal homepage: www.elsevier.com/locate/nimb

Electronic stopping for swift carbon cluster ions connected with average charge reduction

Toshiaki Kaneko *, Kohsuke Ihara, Mahsa Kohno

Graduate School of Science, Okayama University of Science, 1-1 Ridai-cho, Kita-ku, Okayama 700-0005, Japan

ARTICLE INFO

Article history:
Received 6 November 2012
Received in revised form 1 March 2013
Accepted 3 March 2013
Available online 24 March 2013

Keywords:
Cluster ion
Stopping power
Average charge
Dielectric function

ABSTRACT

The cluster effect in the average charge and the electronic energy-loss of swift carbon cluster ions in linear-chained and ring structures with equal separation with kinetic energy ranging from 0.3 to 30 MeV/atom is theoretically investigated on the basis of a recent average charge theory and the dielectric function formalism together with the wave-packet model. The dependence of the cluster average charge on the constituent atoms clearly shows the reductive feature, regardless of the speed, which is more enhanced with increasing the number of constituent atoms. It is proposed that for ring structure, the average charge of constituent ions is determined by an unique self-consistent formula. In the high speed limit it has an asymptotic formula and the reduction effect tends to be vanishing. Regarding the energy loss, the electronic stopping powers of aluminum and silicon targets are calculated for C_n clusters in linear-chain and ring structures with inclusion of the average charge reduction in a bulk. It is found that they show the super-linear cluster effect almost over the range of investigated speed except for large ring clusters at low speed.

1. Introduction

Recently cluster or polyatomic projectiles have attracted intensive interest in the field of investigating the interaction of high energy cluster ions with solid materials both from the basic and applied viewpoints. For example, C60 fullerene ions and highly charged bio-molecules have been accelerated at high energies [1]. From the viewpoints of application, cluster impact has several advantages, e.g., reduction of the kinetic energy per atom and suppression of the charge up effect in ion implantation. From basic viewpoints, on the other hand, it is because the research subjects using polyatomic ion beams are widely ranging, e.g., fragmentation [2–4], multiple ionization [5], emissions of ions and neutrals [6], reduction of average charge [7–9], secondary electron emission [10–13], and energy-deposition to a target [8,14–19], etc. The key term 'cluster effect' originates from a new character of the cluster ion beam, described by the number of constituent atoms and the spatial structure, in addition to the conventional character of the mono-atom ion beam, described by the ion speed, the ion element (or, atomic number), and the distribution of the bound electrons.

The cluster effect was found in the average charge [7–9], the energy-loss phenomena [8,14,16,19–21], and the secondary electron yield [10–13]. As for the average charge, Brunelle et al. [7] found at first the reduction of the cluster average charge per ion. Recently, Chiba et al. [9] reported the structure dependence of the cluster average charge using coulomb explosion imaging technique. They have extended this method to the divergence-angle measurement for various charge-state combinations [22]. Regarding the energy loss of a carbon cluster, there exists the threshold energy around 1 MeV per atom for carbon target. At the incident energies larger than the threshold, the energy loss per ion for a C_n cluster, $\Delta E(n)$, displays the positive or super-linear cluster effect [19], i.e., $D \equiv \Delta E(n) - \Delta E(1) > 0$ or $R \equiv \Delta E(n)/\Delta E(1) > 1$. On the other hand, at lower incident energies, we found a few cases where the negative or sub-linear cluster effect was reported [16]. Recently, making use of a novel experimental method, Tomita et al. [23] clearly observed the sub-linear cluster effect in the energy loss of the 0.5 MeV/atom carbon cluster $C_n^+ (n = 1 - 4)$ penetrating a thin carbon foil. Quite recently, we investigated the cluster average charge and the energy loss of MeV/atom linear-chained C_n clusters penetrating a thin carbon foil in a refined model, which contains the coulomb explosion, the dissipated force, the polarization force, and the average charge reduction in a bulk [24]. It shows the sub-linear and super-linear cluster effects in the energy-loss, respectively, at lower and higher incident energy than the threshold, though the average charge per ion of the clusters indicates the sub-linear effect regardless of high or low ion-speed.

The aim of this paper is to investigate comprehensively the speed dependence of the cluster average charge, and the electronic stopping powers of aluminum and silicon for a C_n cluster with the cluster average charge reduction. Through this paper, m, e and $\hbar$ denote,

* Corresponding author.
E-mail address: kaneko@dap.ous.ac.jp (T. Kaneko).

0168-583X/$ - see front matter © 2013 Elsevier B.V. All rights reserved.
http://dx.doi.org/10.1016/j.nimb.2013.03.025

respectively, the electron rest mass, the elementary charge, and the Planck constant divided by 2π. In addition, the Bohr radius and the Bohr speed are denoted by $a_0 = \hbar^2/(me^2) = 0.529 \times 10^{-10}$ m and v_0 $(= e^2/\hbar) = 2.19 \times 10^6$ m/s, respectively.

2. Theoretical model

2.1. Cluster average charge

It is well known that when energetic ions pass through a solid target, emergent ions have a charge-state distribution, due to subsequent electron capture and loss processes. The average value of the charge states, i.e., average charge, for single-ion incidence is mainly determined by the moving speed, and weakly dependent of material elements. This is supported by the compiled data [25] and the scaling formula holds valid. As for single-ion projectile with atomic number Z, there are several formulas to describe the average charge Q as a function of the speed V, e.g., $Q/Z = a - b\exp(-cV/(Z^d v_0))$. Here a, b, c, d are constant, chosen to fit the experimental data in a scaled form [25], and usually we have $a = b = 1$, $c = 0.8$–1.0 and $d = 2/3$. Insensitive dependence of the average charge on target elements is supposed to come from a strong screening effect of a target-atom potential acting on electron-loss process in a bulk. Recently, based on a fluid-mechanical model, we presented a theoretical formula of the average charge of a single ion with atomic number Z moving in a foil at speed V is given by

$$\frac{Q}{Z} = \frac{2}{\sqrt{\pi}} \int_0^y dt \exp(-t^2), \quad y = \sqrt{\frac{3}{8}} \frac{V}{V_b}, \tag{1}$$

where $V_b = 1.045 Z^{2/3} v_0$ is the average speed of the electrons bound on the ion in a statistical model [10]. This formula implicitly displays that Q/Z is a function of $V/Z^{2/3}v_0$. This expression was extended to cluster-ion projectiles with a modified V_b, which includes the binding effect of surrounding ions via the potential energy. The resultant expression for the average charge Q_i of the ith ion in the cluster is given by

$$\frac{Q_i}{Z} = \frac{2}{\sqrt{\pi}} \int_0^y dt \exp(-t^2),$$
$$y = \sqrt{\frac{3}{8}} \frac{V}{v_0} \left(1.092 Z^{4/3} + 2 \sum_{j(\neq i)}^{n} V_{ji}(R_{ji}) \right)^{-1/2}. \tag{2}$$

Here $V_{ji}(R_{ji})$ denotes the interaction potential energy in atomic units per electron of the ith ion at $\vec{R_i}$ with the jth ion at $\vec{R_j}$. If R_{ji} $(= |\vec{R_j} - \vec{R_i}|)$ is large enough, $V_{ji}(R_{ji})$ reduces to the point-charge value $\frac{Q_j}{R_{ji}}$. Here we give several comments. First, if the inter-atomic separations are large enough, the interaction potential energy term vanishes and consequently the average charge of each ion is determined by its own speed. This means that cluster effect should disappear. The formula (2) reflects this fact clearly. Second, in the limit of very high speed, the average charge of the cluster asymptotically approaches that of a single ion with the corresponding speed. This also means that the cluster effect apparently tends to disappear.

In general, the average charge of each ion depends on the orientation of the cluster and the cluster structure in space. In order to derive general results, however, we neglect the cluster orientation while the cluster is assumed to keep the spatial structure. In spite of this action, we believe that the derived result does not lose a general feature. Let us consider first a cluster in a ring structure, where a 2D ring cluster is composed of n atoms with equal separation of R and the interaction energy is given by in a point charge model as

$$V_{tot} = \sum_{j(\neq i)} V_{ji}(R_{ji}) = \frac{Q}{R} f(n), \quad f(n) = \sum_{j=1}^{n-1} \frac{\sin(\pi/n)}{\sin(j\pi/n)}. \tag{3}$$

It is noted that every ions have the same average charge Q, as is understood from symmetry. Then the average charge in this structure is determined by a self-consistent equation

$$\frac{Q}{Z} = \frac{2}{\sqrt{\pi}} \int_0^y e^{-t^2} dt, \quad y = \sqrt{\frac{3}{8}} \frac{V}{v_0} \left(1.092 Z^{4/3} + \frac{2Q}{R} f(n) \right)^{-1/2}. \tag{4}$$

This is characteristic of a ring-structure cluster. Later we will show numerical results in a few cases for a C_n $(n = 2$–$10)$.

As for linear-chained clusters with equal separation of R, the interaction energy is given by

$$V_i = \sum_{j(\neq i)} V_{ji}(R_{ji}) = \frac{1}{R} \sum_{j(\neq i)} \frac{Q_j}{|j - i|}, \tag{5}$$

so that the upper limit of the integral (2) should be replaced by $y = \sqrt{\frac{3}{8}} \frac{V}{v_0} \left(1.092 Z^{4/3} + \frac{2}{R} \sum_{j(\neq i)}^{n} \frac{Q_j}{|j-i|} \right)^{-1/2}$. Then one find there are more than two different values, depending on the atom position, of the average charge exist for linear-chained C_n $(n > 2)$ clusters. For example, one realizes that the average charge of a central ion in a linear cluster is lower that of an edge ion, comparing the interaction energies for them. We newly call this 'the position effect'. This was supported by a sophisticated experimental data [9]. In this section, we give a theoretical expression in detail for the average charge of a constituent ion in ring and linear-chained clusters. Later, we will depict in several figures the dependence of the calculated cluster average charges on the ion speed, and the position effect.

2.2. Structure factor

In estimating the stopping power of material for a cluster, the spatial structure of a cluster plays a significant role. In cluster impact, we commented that the spatial structure of a cluster is one of important beam parameter. Therefore we briefly describe the structure factor derived from a structure in real space. For simplicity, we represent individual atoms in a cluster composed of n atoms by delta-function points. Then, the spatial distribution of constituent atoms is given by $\rho(\vec{r}) = \sum_{j=1}^{n} \delta(\vec{r} - \vec{R_j})$, so that the structure factor, i.e., the Fourier transform of spatial distribution, is obtained as

$$\rho(\vec{k}) = \int d\vec{r}\, \rho(\vec{r}) \exp(-i\vec{k}\vec{r}) = \sum_{j=1}^{n} \exp(-i\vec{k}\vec{R_j}). \tag{6}$$

The square absolute of the structure factor $\rho(\vec{k})$ is defined here by $S_0(\vec{k})$, so that we obtain

$$S_0(\vec{k}) = |\rho(\vec{k})|^2 = n + \sum_{j}^{n} \sum_{\ell(\neq j)}^{n} \exp(i\vec{k}\vec{R}_{j\ell}), \tag{7}$$

with $\vec{R}_{j\ell} = \vec{R_j} - \vec{R_\ell}$. Here we consider the orientation-averaged quantity $S(k)$ of $S_0(\vec{k})$, then we obtain

$$S(k) = n + \sum_{j}^{n} \sum_{\ell(\neq j)}^{n} \frac{\sin(kR_{j\ell})}{kR_{j\ell}}. \tag{8}$$

This function reflects the spatial structure of a cluster in the Fourier space. Later, one will see the relation between $S(k)$ and the electric stopping power in dielectric formalism.

Fig. 1 shows $S(k)$ as a function of k in atomic units for C_n $(n = 3, 6)$ clusters in a linear-chain and ring structures with equal separation of $2.4a_0$. The solid lines and dashed lines refer to the ring structure and the linear-chain structure, respectively. One can distinguish the curves for C_3 or C_6 by the starting value $S(k = 0) = n^2$.