Charge-Transfer Cross Sections of Slow Doubly and Triply Charged Carbon Ions from CO and CO_2 Molecules*)

Toshio KUSAKABE, Kenji SHIOTA and Toshizo SHIRAI[1)†]

Kinki University, 3-4-1 Kowakae, Higashi-Osaka 577-8502, Japan

[1)]*Japan Atomic Energy Research Institute, Naka-shi, Ibaraki 319-0193, Japan*

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The single- and multiple-charge-transfer cross sections for $^{12}C^{2+}$ and $^{13}C^{3+}$ ions have been measured in collisions with CO and CO_2 molecules in the energy range of 0.35 to 3.0 keV per initial charge number based on the initial growth rate method. Most of the present single- and multiple-charge-transfer cross sections show weak energy dependence over the observed collision energy range. For CO_2 molecules, the present data smoothly join with the previously measured data in the energy range greater than 10 keV. The cross sections for total charge transfer, which are summations of single- and multiple-charge-transfer cross sections, are compared with a simple over-barrier model and available scaling laws.

Keywords: charge-transfer cross section, slow doubly charged carbon ion, slow triply charged carbon ion, carbon monoxide, carbon dioxide, growth rate method, plasma modeling

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1. Introduction

In the edge plasma of recent large tokamak devices with carbon-based plasma-facing materials, low-charge-state carbon ions, many types of carbon containing molecules, and other impurities exist in their plasmas [1, 2]. Among many collision processes relevant to low-temperature fusion edge plasmas, charge-transfer processes of these ions colliding with molecules play a key role in determining the properties of high-temperature core plasmas and in plasma modeling. Therefore, it is very important to accumulate cross section data for charge transfer of carbon ions colliding with various carbon containing molecules.

However, cross section measurements for the C^{q+} (q = 2, 3) + CO and CO_2 collisions are scarce, especially at low collision energies, where q is the initial charge number of the incident ions. At energies greater than 6.3 keV/q, Itoh *et al.* previously measured the cross sections of charge transfer by C^{q+} ions (q = 1 - 4) from CO_2 molecules, together with hydrogen and carbon containing molecules, using a recoil ion source [3]. We also reported preliminary results concerning the dependence of the averaged double-charge-transfer cross sections of C^{2+} ions colliding with various carbon containing molecules on the total number of electrons in the target molecules [4].

In this study, we present the single- and multiple-charge-transfer cross sections, $\sigma_{q,q-k}$, of C^{q+} ions (q = 2, 3) in collisions with CO and CO_2 molecules in the energy range between 0.35 and 3.0 keV/q, where k is the final number of electrons transferred from target molecules. These cross section values are compared with the previous data. Since we observed the final charge states of primary ions passing through the target gas, our "k –charge transfer" cross section, $\sigma_{q,q-k}$, for the final $(q-k)$+ ions includes both radiative and Auger processes. The cross section for total charge transfer, which means the summation of cross sections for all possible numbers of transferred electrons, is given by

$$\sigma_{\rm tot} = \sum_{k\geq 1} \sigma_{q,q-k}. \quad (1)$$

Scaling properties of the present cross sections for total charge transfer are also discussed.

2. Experimental

A detailed description of the experimental apparatus and methods used in the present study has been previously given [4–8]. Some important points and differences from the previous study are briefly mentioned here.

Doubly and triply charged carbon ions were produced from high-purity CO_2 or CH_4 gaseous molecules by impacting on an electron beam of 2 keV and approximately 1 mA emitted from a barium-oxide cathode in a compact electron beam ion source called micro-EBIS [9] using a strong ring permanent magnet. To avoid contamination of $^{16}O^{4+}$ ions, enriched ^{13}CO or $^{13}CH_4$ gases were used to produce $^{13}C^{3+}$ ions.

Then, the $^{12}C^{2+}$ and $^{13}C^{3+}$ ion beams were mass-separated with a Wien filter and introduced into a 40-mm-long collision cell, which was filled with target gases

author's e-mail: kusakabe@phys.kindai.ac.jp

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† deceased

of more than 99.95 % purity. The target gas pressure in the collision cell was measured with a calibrated high-sensitivity Pirani gauge and ranged from 0.005 to 0.3 Pa. After the charge-transfer collisions, the charged and neutral carbon particles emerging from the cell were separated with an electrostatic deflector and detected with a position-sensitive micro-channel plate detector (MCP-PSD). The cross sections of charge transfer were determined on the basis of an initial growth rate method: that is, the cross sections were determined from the slope of the linear part of the observed fraction curves for product carbon ions and atoms formed in charge-transfer collisions versus the target gas thickness. It is assumed that the detection efficiencies of the present MCP-PSD for C^{3+}, C^{2+}, C^+ and C particles are identical within the experimental uncertainties over the present collision energy range, as discussed in previous studies [10–12]. The vacuum system was evacuated with two turbo-molecular pumps (50 and 500 l/s) and a cryogenic pump. The typical residual gas pressure was approximately 5×10^{-7} Pa in the vacuum chambers containing the micro-EBIS.

The statistical and systematic uncertainties of the observed single- and multiple-charge-transfer cross sections were separately determined. As a result, total experimental uncertainties of the absolute cross sections are given as the quadratic sum of these uncertainties, and they range from 10.6 to 16.7 %.

3. Results and Discussion

3.1 C^{2+} ion collisions

The present experimental cross sections for single- and double-charge transfer by C^{2+} ions colliding with CO and CO_2 molecules are listed in Tables 1 and 2, respectively.

The present experimental charge-transfer cross sections of C^{2+} ions in collisions with CO molecules are shown in Fig. 1. The energy dependence of the present $\sigma_{2,1}$ data is very weak, and their average value is 2.06×10^{-15} cm^2. The present $\sigma_{2,0}$ data are decreasing gradually as collision energy increases, and those averaged value is 3.11×10^{-16} cm^2.

The present experimental charge-transfer cross sections of C^{2+} ions in collisions with CO_2 molecules are shown in Fig. 2 together with the previous data of Itoh *et al.* [3]. As the collision energy increases, the present $\sigma_{2,1}$ values slightly increase, while the present $\sigma_{2,0}$ values decrease. They can then be smoothly joined with the data of Itoh *et al.* [3] at energies greater than 10 keV. The energy dependence of both cross sections is weak, and their average values are 2.29×10^{-15} and 4.85×10^{-16} cm^2, respectively.

3.2 C^{3+} ion collisions

The present experimental cross sections for single- and double-charge transfer by C^{3+} ions colliding with CO and CO_2 molecules are listed in Tables 3 and 4, respectively.

The present experimental charge-transfer cross sections of C^{3+} ions in collisions with CO molecules are shown in Fig. 3. The energy dependence of the present $\sigma_{3,2}$ and $\sigma_{3,1}$ data is very weak, and their average values are 1.09×10^{-15} and 1.19×10^{-15} cm^2, respectively. In the energy range greater than 4 keV, both the present $\sigma_{3,2}$ and $\sigma_{3,1}$ values are almost the same. At energies below 3 keV, the $\sigma_{3,2}$ values become smaller than the $\sigma_{3,1}$ values as collision energy decreases. The present $\sigma_{3,0}$ values gradually decrease as collision energy increases, and their average

Table 1 Cross sections of single- and double-charge transfer by C^{2+} ions from CO molecules.

Energy (keV)	Cross section ($\times 10^{-16}$ cm^2)	
	$\sigma_{2,1}$	$\sigma_{2,0}$
0.70	21.7 ± 3.1	4.45 ± 0.63
1.5	20.3 ± 2.5	2.97 ± 0.36
3.0	19.7 ± 2.2	2.53 ± 0.28
6.0	20.6 ± 2.3	2.49 ± 0.27

Table 2 Cross sections of single- and double-charge transfer by C^{2+} ions from CO_2 molecules.

Energy (keV)	Cross section ($\times 10^{-16}$ cm^2)	
	$\sigma_{2,1}$	$\sigma_{2,0}$
0.70	20.6 ± 2.9	5.99 ± 0.83
1.5	21.1 ± 3.0	4.83 ± 0.67
3.0	24.9 ± 3.0	4.52 ± 0.54
6.0	25.0 ± 2.7	4.07 ± 0.45

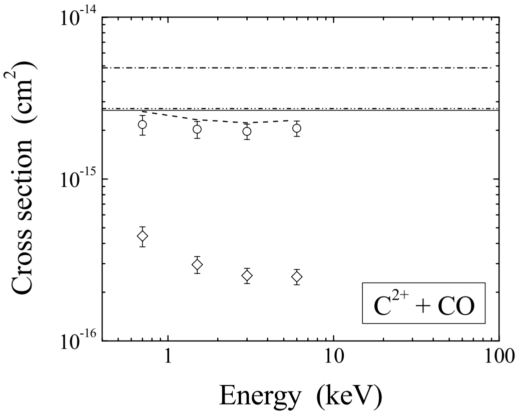

Fig. 1 Single- and double-charge-transfer cross sections of C^{2+} ions colliding with CO molecules. Experimental data: ○, present $\sigma_{2,1}$ data; ◇, present $\sigma_{2,0}$ data; -----, present σ_{tot} data. Scaling law: dot-dashed line, CASM [13]; solid line, MK [14]; dot-dot-dashed line, TK [8].

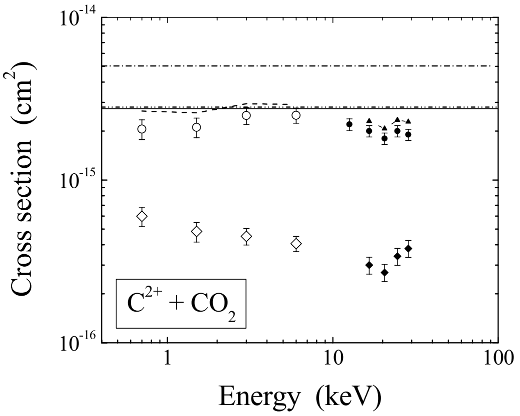

Fig. 2 Single- and double-charge-transfer cross sections of C^{2+} ions colliding with CO_2 molecules. Experimental data:○, present $\sigma_{2,1}$ data; ◇, present $\sigma_{2,0}$ data; -----, present σ_{tot} data; ●, $\sigma_{2,1}$ data of Itoh *et al.* [3]; ◆, $\sigma_{2,0}$ data of Itoh *et al.* [3]; --▲--, σ_{tot} data of Itoh *et al.* [3]. Scaling law: dot-dashed line, CASM [13]; solid line, MK [14]; dot-dot-dashed line, TK [8].

Table 3 Cross sections of single-, double- and triple-charge transfer by C^{3+} ions from CO molecules.

Energy (keV)	Cross section (× 10^{-16} cm^2)		
	$\sigma_{3,2}$	$\sigma_{3,1}$	$\sigma_{3,0}$
1.05	9.4 ± 1.5	12.4 ± 1.9	1.51 ± 0.24
2.25	11.3 ± 1.5	12.5 ± 1.6	1.12 ± 0.15
4.50	10.9 ± 1.4	11.2 ± 1.4	0.91 ± 0.12
9.00	12.0 ± 1.7	11.6 ± 1.5	0.90 ± 0.15

Table 4 Cross sections of single-, double- and triple-charge transfer by C^{3+} ions from CO_2 molecules.

Energy (keV)	Cross section (× 10^{-16} cm^2)		
	$\sigma_{3,2}$	$\sigma_{3,1}$	$\sigma_{3,0}$
1.05	6.8 ± 1.0	15.3 ± 2.1	2.25 ± 0.32
2.25	8.8 ± 1.1	15.1 ± 1.8	1.86 ± 0.23
4.50	9.2 ± 1.1	14.4 ± 1.6	1.81 ± 0.21
9.00	10.2 ± 1.2	14.5 ± 1.6	1.55 ± 0.17

value is 1.11×10^{-16} cm^2.

The present experimental charge-transfer cross sections of C^{3+} ions in collisions with CO_2 molecules are shown in Fig. 4 together with the previous measurements of Itoh *et al.* [3]. As the collision energy increases, the present $\sigma_{3,2}$ values increase, whereas the present $\sigma_{3,1}$ and $\sigma_{3,0}$ values slightly decrease. They can then be smoothly joined with the data of Itoh *et al.* [3] at energies greater than 20 keV. Surprisingly, the present $\sigma_{3,2}$ values are apparently smaller than the present $\sigma_{3,1}$ values over the entire studied energy range. The energy dependence of both $\sigma_{3,1}$ and $\sigma_{3,0}$ data is very weak, and their average values are 1.48×10^{-15} and 1.87×10^{-16} cm^2, respectively. The average value of the $\sigma_{3,2}$ data is 8.74×10^{-16} cm^2.

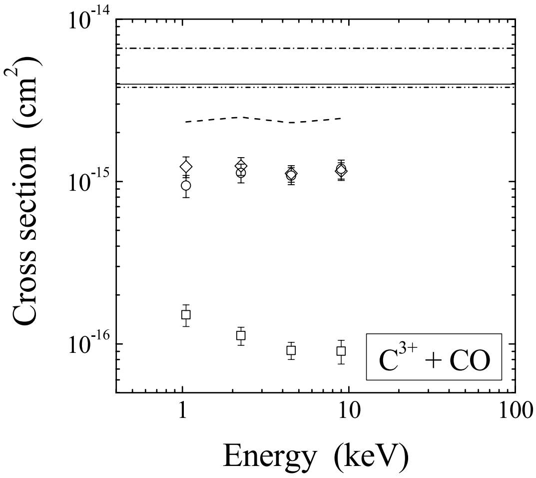

Fig. 3 Single-, double- and triple-charge-transfer cross sections of C^{3+} ions colliding with CO molecules. Experimental data: ○, present $\sigma_{3,2}$ data; ◇, present $\sigma_{3,1}$ data; □, present $\sigma_{3,0}$ data; -----, present σ_{tot} data. Scaling law: dot-dashed line, CASM [13]; solid line, MK [14]; dot-dot-dashed line, TK [8].

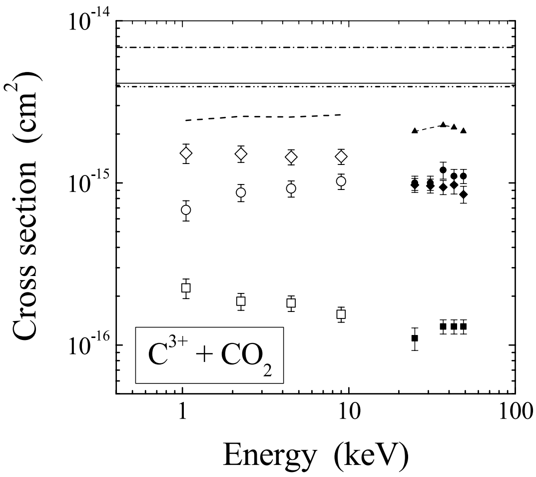

Fig. 4 Single-, double- and triple-charge-transfer cross sections of C^{3+} ions colliding with CO_2 molecules. Experimental data: ○, present $\sigma_{3,2}$ data; ◇, present $\sigma_{3,1}$ data; □, present $\sigma_{3,0}$ data; -----, present σ_{tot} data; ●, $\sigma_{3,2}$ data of Itoh *et al.* [3]; ◆, $\sigma_{3,1}$ data of Itoh *et al.* [3]; ■, $\sigma_{3,0}$ data of Itoh *et al.* [3]; --▲--, σ_{tot} data of Itoh *et al.* [3]. Scaling law: dot-dashed line, CASM [13]; solid line, MK [14]; dot-dot-dashed line, TK [8].

3.3 Total charge-transfer cross sections

In Figs. 1–4, dashed lines indicate the present experimental cross sections for total charge transfer.

According to a classical over-barrier model for a projectile ion with quasi-continuous energy levels, which was called the "classical absorbing-sphere model" (CASM) treated by Janev and Presnyakov [13], a target electron can pass over the potential barrier at a critical inter-nuclear distance R_c. The cross section for total charge transfer is then given by

$$\sigma_{tot}^{CASM} = \pi R_C^2 = \pi(2\sqrt{q} + 1)^2 I_1^{-2}, \tag{2}$$

where I_1 is the first ionization potential of target particles. For $q \gg 1$, the expression σ_{tot}^{CASM} can be approximated as follows:

$$\sigma_{tot}^{MK} = 4\pi q I_1^{-2}. \tag{3}$$

In case of total charge transfer, this expression is identical to the scaling law proposed by Kimura *et al.* [14] based on an extended classical over-barrier model [15].

Kusakabe *et al.* [8] previously presented the cross sections of total charge transfer by $2q$ keV Ne^{q+} (q = 2 - 6) and Ar^{q+} (q = 2 - 9) ions colliding with various hydrocarbon molecules, and gave the following best fit relation:

$$\sigma_{tot}^{TK} = 1.56 \times 10^{-13} \cdot q^{0.825} \cdot I_1^{-1.75} \quad [\mathrm{cm}^2], \tag{4}$$

was given where I_1 is expressed in units of eV.

In Figs. 1 - 4, the dot-dashed, solid, and dot-dot-dashed lines represent the CASM [13], the scaling law proposed by Kimura *et al.* [14], and the empirical scaling relation reported by Kusakabe *et al.* [8], respectively. It is thought that the CASM gives the possible upper limit of the total charge-transfer cross sections. The σ_{tot}^{TK} values are very close to the σ_{tot}^{MK} TK values. For C^{2+} ions, both σ_{tot}^{TK} and σ_{tot}^{MK} values are very close to the present experimental σ_{tot} data. While both σ_{tot}^{TK} and σ_{tot}^{MK} values are approximately 1.7 times as large as the present experimental σ_{tot} data for C^{3+} ions.

In conclusion, the present observations have provided reasonably reliable cross section data for the charge transfer of $^{12}C^{2+}$ and $^{13}C^{3+}$ ions in collisions with CO and CO_2 molecules in the energy range below $3q$ keV. Most of the present single- and multiple-charge-transfer cross sections show weak energy dependence over the observed collision energy range. The $\sigma_{2,0}$, $\sigma_{3,1}$, and $\sigma_{3,0}$ cross section data gradually decrease as collision energy increases. This energy dependence is characterized by a so-called resonant charge-transfer reaction. Although the direct multiple-charge transfer to a carbon atom is an endothermic reaction for CO and CO_2 targets, the double-charge transfer of C^{3+} ions and single-charge transfer can consider various exothermic reactions with many vibrational excited states of product target molecular ions. In the step-by-step process of the charge transfer via single- or/and double-charge transfer, a critical radius of charge transfer may be expanded and then cross section value becomes large, and finally it is expected to cause about this energy dependence.

It should be emphasized that it will also be important to determine the cross sections at still much lower energies, which may be critical in the diverter region.

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