Cross Sections of Charge Transfer by Slow Doubly-Charged Carbon Ions from Various Carbon Containing Molecules

KUSAKABE Toshio, SHIOTA Kenji, KUBO Hirotaka¹ and SHIRAI Toshizo^{1*}

Department of Science, Kinki University, Higashi-osaka 577-8502, Japan ¹ Naka Fusion Research Establishment, Japan Atomic Energy Research Institute, Ibaraki 311-0193, Japan (Received: 5 October 2004 / Accepted: 20 December 2005)

Abstract

The single- and double-charge transfer cross sections for doubly-charged C^{2+} ions have been measured in collisions with CO, CO₂, CH₄, C₂H₂, C₂H₄, C₂H₆, C₃H₄ (allene), C₃H₄ (propyne), C₃H₆, (CH₂)₃, C₃H₈, n-C₄H₁₀ and i-C₄H₁₀ molecules in the energy range of 0.70 to 6.0 keV using the initial growth rate method. Most of the present single- and double-charge transfer cross sections are found to show a weak energy dependence over the observed collision energy range. The single-charge transfer cross sections for hydrocarbons depend on the first ionization potential of the target molecules. On the other hand, for the double-charge transfer cross sections, such a simple dependence on the first ionization potential cannot be found, while a fairly good systematic dependence of the double charge transfer cross sections is found on the total number of electrons in the target molecules. Moreover, the present double-charge transfer cross sections decrease with the increasing collision energy. This feature indicates that the vibrational excited states of the target molecular ions produced after charge transfer might have resulted in the creation of near or accidentally resonant reaction channels. Based on this viewpoint, a new empirical scaling relation for the double-charge transfer cross sections is derived.

Keywords:

charge transfer cross section, slow doubly-charged carbon ion, carbon containing molecule, double-charge transfer, accidental resonant reaction, empirical scaling relation

1. Introduction

In current and next day large tokamaks with carbonbased plasma-facing materials, carbon ions and many kinds of carbon containing molecules as well as other impurities exist in their edge and divertor plasmas [1, 2]. For understanding the impurity behavior, cross section data for the charge transfer processes of these ions with molecules are required.

Many investigations have been performed on the charge transfer of ions in collisions with various atoms and molecules up to the present time. To our knowledge, however, only one data set is available for the collisions of C^{2+} ions with carbon containing molecules. Itoh *et al.* measured the cross sections of charge transfer by C^{2+} ions from CO₂, CH₄, C₂H₆ and C₃H₈ at energies from 12.6 to 32.6 keV using a recoil ion source [3].

We have measured the single- and double-charge transfer cross sections, σ_{21} and σ_{20} , of C²⁺ ions in collisions with CO, CO₂, and various hydrocarbons (CH₄, C₂H₂, C₂H₄, C₂H₆, C₃H₄ (allene), C₃H₄ (propyne),

 C_3H_6 , $(CH_2)_3$, C_3H_8 , $n-C_4H_{10}$, $i-C_4H_{10}$) in the energy range of 0.70 to 6.0 keV. In this paper, the dependence of these double-charge transfer cross sections on the total number of electrons in the target molecules is discussed and a simple empirical scaling relation is presented.

2. Experimental

The experimental apparatus and methods used in the present study are essentially the same as the previous ones [4-7]. However, some important points and differences from the previous study are briefly mentioned here.

Doubly-charged carbon ions were produced from high purity CO_2 or CH_4 gases by impacting on about a 1 mA and 2 keV electron beam emitted from a barium oxide cathode in a compact electron beam ion source called micro-EBIS [8] using a strong ring permanent magnet. The mass-analyzed C^{2+} ions with a Wien filter were then passed through a 40 mm long collision cell.

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

Target gases of high purity (> 99.5%, except C₃H₄ (Allene; 97 % and Propyne; 98 %)) were used and the pressure in the collision cell was measured by a calibrated Pirani gauge. After the charge-transfer collisions, the charged and neutral particles emerging from the cell were separated by an electrostatic deflector and detected with a position-sensitive microchannel plate multiplier. Their fractions were determined from the peak areas in the charge spectrum recorded on a multichannel pulse height analyzer as a function of the target gas thickness π , based on the growth rate method. The observed fractions, F_i , were separately fitted to a quadratic function $(a_i\pi + b_i\pi^2)$ and fitting parameters, a_i , correspond single- and double-charge transfer cross sections, $\sigma_{2i}(j = 1, 0)$, respectively. The residual gas pressure was about 1×10^{-6} Pa in the whole vacuum chambers containing the micro-EBIS and the collision cell, which were exhausted with two turbo-molecular pumps (500 l/s and 50 l/s) and a cryo-pump.

The statistical and systematic uncertainties of the observed single- and double-charge transfer cross sections, σ_{21} and σ_{20} , are separately determined. The statistical uncertainties of the cross sections are between 0.275 and 8.47% for all of the present results. Systematic uncertainties due to the determination of sensitivity coefficient of the Pirani gauge, target thickness, the temperature of the target gases, charge separation on the position spectrum of the MCP-PSD and so forth are estimated to range from 10.7% at high energies to 16.3% at low energies. The total experimental uncertainties of the absolute cross sections are given as the quadratic sum of the involved uncertainties.

3. Results and discussion

3.1 Dependence of cross sections on incident energy

The single- and double-charge transfer cross sections of the C²⁺ ions in collisions with CH₄ molecules are shown in Fig.1, as an example, together with the previous data of Itoh *et al.* [3]. As the collision energy increases, the present single-charge transfer cross sections increase, while the present double-charge transfer cross sections decrease. At even high energies, they can be then smoothly connected with the data of Itoh *et al.* [3]. The energy dependences of both cross sections are very weak. For most of the other molecules, similar energy dependencies on the incident energy to methane are shown. However, the present σ_{21} data for CO, C₃H₄ (allene), C₃H₄ (propyne), (CH₂)₃, and i-C₄H₁₀ molecules are found to be almost constant.

Generally, the charge transfer of doubly-charged ions can possibly make an exothermic reaction chan-



Fig. 1 Single- and double-charge transfer cross sections for C^{2+} ions in collisions with CH_4 molecules.

nel. The exothermic reactions can make some vibrationally excited states and dissociation of the product target molecular ions, and result in the creation of an accidental resonant charge transfer. In the case of the resonant charge transfer of singly-charged ions, their cross sections gradually decrease with the increasing incident energy. The cross section σ for these processes is given by

$$\sigma = (a - b \cdot \log v)^2, \tag{1}$$

where a and b are constants and v is the velocity of the incident ions [9, 10]. It is found that this formula can fit the present double-charge transfer cross sections. This will be discussed in the following subsection.

3.2 Dependence of cross sections on total number of electrons in target molecules

Finding some scaling relations for the cross sections of charge transfer is useful for application to other fields of science and technology. Generally, the dependence on the first ionization potential I_1 (eV) of target molecules is frequently examined for the charge transfer cross sections of slow ions. The present σ_{21} data for hydrocarbons, except the CO and CO₂ molecules, are found to definitely depend on first ionization potential and to lie around the empirical scaling relation of Kusakabe *et al.* [11] derived by 0.286 keV Kr^{*q*+}($q = 2 \sim 9$) and Xe^{*q*+}($q = 2 \sim 11$) ions colliding with some rare gas atoms and simple molecules, which was represented by $\sigma_{21} = 9.5 \times 10^{-14} \cdot q^{1.3} \cdot I_1^{-2.0}$ [cm²]. For the present σ_{20} data, however, a simple relation to I_1 could not be determined.

As for the total number of electrons, N_E , the polarizability, the number of bonds in the hydrocarbons and the



Fig. 2 Dependence of averaged double-charge transfer cross sections for C²⁺ ions in collisions with various carbon containing molecules on the total number of electrons. Solid line is the best fit of the present data (eq. (2)).

length of the hydrocarbon molecules are representative parameters related to the "molecular size". We have examined the dependences on these parameters and fairly good systematic dependences of the present σ_{20} data on the total number of electrons, the polarizability, and the number of bonds in target molecules were observed. In this paper, the dependence of the averaged present cross sections of the double-charge transfer on the total number of electrons N_E is shown in Fig. 2. A fairly good concentration can be seen for the hydrocarbons, except for the CO and CO₂ molecules. For the present averaged $\langle \sigma_{20} \rangle$ cross sections for hydrocarbons, a best fit relation

$$\langle \sigma_{20} \rangle = 7.2 \times 10^{-17} \cdot N_E \quad (\text{cm}^2)$$
 (2)

is obtained and is represented by the solid line in Fig.2.

Combining eq. (2) with eq. (1), we propose the following empirical relation for the double-charge transfer cross sections of C^{2+} ions in collisions with hydrocarbons:

$$\sigma_{20} = 8.1 \times 10^{-17} \cdot (1 - 0.15 \cdot \log_{10} E)^2 \cdot N_E \quad (\text{cm}^2) \quad (3)$$

where *E* is the kinetic energy of the incident ions in keV. Figure 3 shows the reduced plot (σ_{20}/N_E values) of the double-charge transfer cross sections versus incident energy *E*. A good correlation of the experimental data for the hydrocarbons to eq. (3) can be seen in



Fig. 3 Reduced plot of double-charge transfer cross sections for C²⁺ ions in collisions with various hydrocarbons.

Fig. 3. The following approximated relation is a simpler form and also applicable.

$$\sigma_{20} = 8.1 \times 10^{-17} \cdot E^{-0.15} \cdot N_E \quad (\text{cm}^2) \tag{4}$$

A detailed description of the single-charge transfer cross sections and dependences of the double-charge transfer cross sections on other molecular constants, such as the polarizability and the number of bonds, will be discussed elsewhere.

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