Electron Capture Processes in Low Energy Collisions of C^{4+} Ions with Excited H Atoms

SHIMAKURA Noriyuki, HONMA Mayumi[1] and KUBO Hirotaka[2]

Faculty of Science, Niigata University, Niigata 950-2181, Japan

[1] *Graduate School of Science and Technology, Niigata University, Niigata 950-2181, Japan*

[2] *Japan Atomic Energy Research Institute, Naka 311-0193, Japan*

Abstract

Cross sections for electron capture in collisions of C^{4+} ions with H*($n = 2$) atoms have been calculated using a molecular-basis close-coupling method in the collision energy range from 60 eV/amu to 6 keV/amu. The calculated results show that electrons are dominantly captured in the $n = 6$ states of the C^{3+} ions and the maximum of the total cross sections is about 900×10^{-16} cm^2 and 600×10^{-16} cm^2 in the C^{4+}(1s^2) + H*(2s) and C^{4+}(1s^2) + H*(2p) collisions, respectively.

Keywords:

1. Introduction

It has recently been recognized that in tokamak divertors, emission from $n = 6$ and 7 states of C^{3+} ions is sometimes quite strong and hence the measurement of spectral lines from C^{3+} ($n = 5, 6, 7$) ions is appropriate for study of carbon impurity behavior [1,2]. It is anticipated that the C^{3+} ($n = 5, 6, 7$) ions are mainly produced by electron capture by C^{4+} ions from excited H*($n = 2$) atoms. Therefore, the cross sections for electron capture are needed for analysis of the spectroscopic measurements. The cross sections for electron capture in collisions of C^{4+} ions with ground H atoms have been obtained by Bliek *et al.* [3] experimentally and by Tseng and Lin [4] and Errea *et al.* [5] theoretically. However, no estimation has been performed for the case of excited H*($n = 2$) atoms except for classical trajectory Monte Carlo (CTMC) calculations by Zaniol *et al.* [1] at a collision energy of 1 eV/amu. On the other hand, Macek and Ovchinnikov [6] developed a simple model for electron capture from high n states of H atoms by multiply-charged ions and predicted that the cross sections depend upon n as n^5. They have insisted that this high n dependence explains why a small fraction (less than 0.1 %) of hydrogen in high n states contributes 30 % of the capture yield at 50 eV/amu in O^{5+} + H collisions. Combining this model with the cross sections for the ground H atoms, we can anticipate that the cross sections for the excited H atoms have maximum value of about 1000×10^{-16} cm^2.

In this paper, cross sections for electron capture in collisions of C^{4+} ions with H*($n = 2$) atoms have been calculated using a molecular-basis close-coupling method [7] in the collision energy range from 60 eV/amu to 6 keV/amu.

2. Calculation method

Since the details of the theoretical treatment in this paper have already been described [7], only the specific information used for the present calculation is given below.

2.1 Electronic states and couplings

The electronic structures were calculated using a generalized valence-bond configuration-interaction (CI) method with l-dependent Gaussian-type pseudo-potential representing the C^{4+}(1s^2) ion. Hence only one active electron was treated explicitly. The pseudo-potential parameters were taken from the paper by Kimura and Olson [8]. In the CI calculations, Slater-type orbitals (STOs) were used to construct basis sets. The orbital exponents of the STOs were obtained by optimizing the energies of the respective electronic states. The accuracy of the present electronic state calculations with respect to the spectroscopic values [9] is better than 0.05 eV except for the C^{3+}(2s) and C^{3+}(3s) states, these two states contributing only little to the electron capture.

We calculated the radial and rotational couplings

Corresponding author's e-mail: shima@shimakura.gs.niigata-u.ac.jp

Table 1　Partial n-shell cross sections (in 10^{-16} cm^2) in C^{4+} + H*($n=2$) collisions calculated with basis set A.

E (keV/amu)	0.248	0.558	0.992	1.550	3.038	5.022	6.200
C^{3+}($n=2$)	0.018	0.022	0.079	0.231	0.417	0.820	0.952
C^{3+}($n=3$)	0.630	1.490	2.646	5.443	5.076	4.276	5.263
C^{3+}($n=4$)	4.504	5.031	6.894	7.582	9.478	8.458	7.711
C^{3+}($n=5$)	32.22	33.53	36.68	26.79	41.32	40.19	40.66
C^{3+}($n=6$)	182.3	189.2	180.6	184.0	170.3	141.3	137.2
C^{3+}($n=7$)	112.6	125.7	125.0	113.4	133.9	131.5	126.2
C^{3+}($n=8$)	8.955	18.25	24.15	16.36	11.96	14.62	14.12

with atomic-type electron translation factors (ETFs) to solve the close-coupling equations. The ETFs were included to the first order in velocity.

2.2　Collision dynamics

A semi-classical molecular-state close-coupling method was employed at collision energies from 60 eV/amu to 6 keV/amu. The coupled equations were solved numerically under the assumption of straight-line trajectories for the heavy-particle motion. By squaring the resulting amplitude, the transition probability was obtained as a function of collision energy and impact parameter. The cross sections were given by an integration of impact-parameter-weighted transition probability over the impact parameter.

3.　Results and discussion

The close-coupling calculations were performed using two kinds of basis sets. One basis set (basis set A) includes 31 channels of only Σ states from C^{3+}($1s^2nl$; nl = 2s, 2p, 3s – 3d, 4s – 4f, 5s – 5g, 6s – 6h, 7s – 7i, 8s) + H$^+$ and C^{4+}($1s^2$) + H (1s, 2s, 2p) states and the other (basis set B) includes 58 channels of Σ, Π, Δ, and Φ states from C^{3+}($1s^2nl$; nl = 5s – 5g, 6s – 6h, 7s – 7i, 8s) + H$^+$ and C^{4+}($1s^2$) + H (1s, 2s, 2p) states.

3.1　Cross sections with basis set A

Calculations for the C^{4+}($1s^2$) + H (2s) and C^{4+}($1s^2$) + H (2p) collisions were performed separately. Table 1 shows the partial n-shell cross sections obtained by summing the calculated cross sections for the C^{4+}($1s^2$)+ H (2s) and C^{4+}($1s^2$) + H (2p) collisions with statistical weights. This table shows that the most dominant states for the electron capture processes are the n = 6 states and the second dominant ones are the n = 7 states. The sum of the contributions from the two states amounts to about 90 % of the total cross sections over the collision energies treated in this paper. At higher collision energies, the contributions of the n = 6 states decrease slowly with the collision energy and the contributions of the second dominant n = 7 states become comparable

to the first dominant ones. The results by CTMC calculations has also shown that the most dominant states were the n = 6 states, but the second dominant ones was the n = 5 states at the collision energy of 1 eV/amu [1]. Both our calculated results and CTMC results show that the contributions of the C^{3+}($1s^2nl$; n = 2, 3, 4) + H$^+$ states to the electron capture are less than 3 % of the total cross sections.

3.2　Cross sections with basis set B

As described in the above paragraph, the C^{3+}($1s^2nl$; n = 2, 3, 4) + H$^+$ states scarcely contribute to the electron capture under the condition calculated in this paper. So, we next performed the close-coupling calculations with the basis set B, in which not only the Σ states but also Π, Δ, and Φ states were included instead of the above-mentioned non-effective Σ states. The obtained results are shown in Figs. 1 and 2 for the C^{4+}($1s^2$) + H*(2s) and C^{4+}($1s^2$) + H*(2p) collisions, respectively. In order to confirm the convergence of the cross sections to the size of basis set, we also performed the calculations removing nine Φ states from the basis set B for the C^{4+}($1s^2$) + H*(2s) collisions. The solid and broken curves in Fig. 1 show the cross sections calculated with and without the Φ states, respectively. Both results
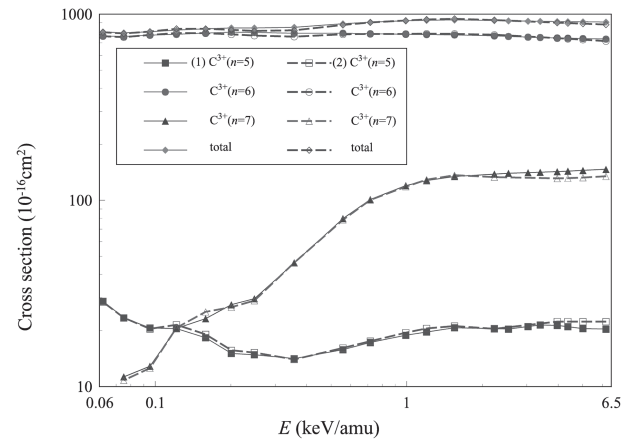
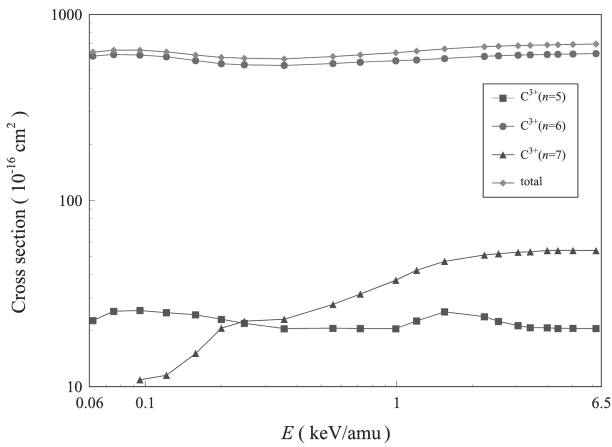Fig. 1　Cross sections for the electron capture in the C^{4+} + H* (2s) collisions.

Fig. 2   Cross sections for the electron capture in the C^{4+} + H*(2p) collisions.

Fig. 3   Total cross sections for the electron capture in the C^{4+} + H(1s) and C^{4+} + H*(2l) collisions.

are similar each other, so we can conclude that only the Σ, Π, and Δ states contribute to the electron capture processes. In Fig. 2, the partial n-shell and total cross sections are shown for the C^{4+}(1s^2) + H*(2p) collisions. The general trend of the cross sections for the C^{4+}(1s^2) + H*(2p) collisions is similar with that for the C^{4+}(1s^2) + H*(2s) collisions, but the cross sections for the former are a little smaller than those for the latter. As the case of basis set A, the most dominant states are the n = 6 states over the collision energies treated in this paper and the second dominant states are the n = 7 states at higher collision energies. However, at lower collision energies the n = 7 states change off with the n = 5 states. Our results also show that the captures into lower angular momentum states dominate at low collision energies (E < 10 keV/amu), but at higher collision energies the contributions of the each angular momentum states become close to the statistical weight.

3.3   The comparison of the cross sections calculated for the C^{4+} + H*(2l) collisions with the cross sections for the C^{4+} + H(1s) collisions

In Fig. 3, all the available total cross sections for the electron capture in the C^{4+} + H(1s) and C^{4+} + H*(2l) collisions are compared except for one calculation by CTMC method at very low collision energy. Three groups have reported the cross sections for the electron capture in the C^{4+} + H(1s) collisions [3 − 5]. There is about 30 % discrepancy among them, but roughly speaking all the total cross sections give maximum values of about 30×10^{-16} cm^2 at collision energy of about 250 eV/amu. On the other hand, the total cross section obtained by CTMC method for the C^{4+}(1s^2)+H*(n = 2) collisions is about 380×10^{-16} cm^2 at a collision energy of 1 eV/amu. This value is pretty large, but is not
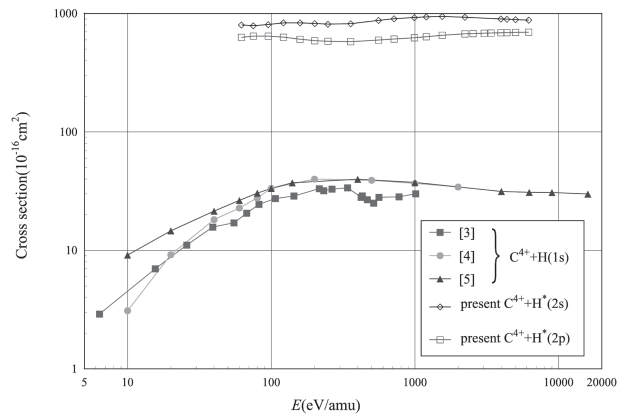
so large compared with the value of 1000×10^{-16} cm^2 which is anticipated by the Macek-Ovchinnikov model using the maximum value for the C^{4+} + H(1s) collisions. On the other hand, as described in the above paragraph, our molecular-basis close-coupling calculations show that the total cross sections reach maximum values of about 900×10^{-16} cm^2 and 600×10^{-16} cm^2 for the C^{4+}(1s^2) + H*(2s) and C^{4+}(1s^2) + H*(2p) collisions, respectively. The classical method like CTMC does not seem to be good at low collision energy of 1 eV/amu, but in order to obtain more definite results about this point, we are performing full quantum calculations at low collision energies. We can explain the reason why the cross sections for the C^{4+}(1s^2) + H*(2l) collisions is so large, as follows. The electrons in the H*(2l) states distribute more widely than that in the H(1s) state, so the C^{4+} ions can capture the electrons in the H*(2l) states even at larger distances compared with the case of the H(1s) states. For the C^{4+} + H(1s) collisions, the electrons are mainly captured into the C^{3+}(3l) states and the region of the effective avoided crossing for the electron capture is $6.5 \leq R_C(au) \leq 8.0$. On the other hand, for the C^{4+}(1s^2) + H*(2l) collisions, the electrons are mainly captured into the C^{3+}(6l) states and the region of the effective avoided crossing is $20.0 \leq R_C(au) \leq 30.0$. At lower collision energies, the transitions are localized in the neighborhood of the avoided crossing points, so only the C^{3+}(6l) + H$^+$ states contribute mainly to the electron capture. However, with increasing the collision energy, the electron capture occurs also at a wide region of internuclear distances away from the avoided crossing points, so the cross section for electron capture into the C^{3+}(7l) states gradually becomes large.

References

[1] B. Zaniol, R.C. Isler, N.H. Brooks, W.P. West and R.E. Olson, Phys. Plasmas **8**, 4386 (2001).

[2] T. Nakano, H. Kubo, N. Asakura, K. Shimizu and S. Higashijima, J. Plasma Fusion Res. **80**, 500 (2004).

[3] F.W. Bliek, R. Hoekstra, M.E. Bannister and C.C. Havener, Phys. Rev. A **56**, 431 (1997).

[4] H.C. Tseng and C.D. Lin, Phys. Rev. A **58**, 1966 (1988).

[5] L.F. Errea, J.D. Gorfinkiel, C. Harel, H. Jouin, A. Macias, L. Mendz, B. Pons and A. Riera, J. Phys. B **32**, L673 (1999).

[6] J. Macek and S.Y. Ovchinnikov, Phys. Rev. Lett. **69**, 2357 (1992).

[7] M. Kimura and N.F. Lane, *Advances in Atomic, Molecular, and Optical Physics*, edited by D. R. Bates and B. Bederson (Academic, New York, 1989), Vol. **26**, p. 79.

[8] M. Kimura and R.E. Olson, J. Phys. B：At. Mol. Opt. Phys. **17**, L713 (1984).

[9] S. Bashkin and J.R. Stoner, J.R. Jr., *Atomic Energy levels and Grotrian Diagrams I* (North-Holland, Amsterdam, 1975).