

Investigation on Collision of Si^{2+} with H from Intermediate to High Projectile Energies

B. He^{1,*}, J. G. Wang¹, C. L. Liu¹, Y. Ning¹, Y. B. Qiu¹, J. Yan¹
and P. C. Stancil²

¹ *Key Laboratory of Computational Physics, Institute of Applied Physics and Computational Mathematics, Beijing 100088, P. R. China.*

² *Department of Physics and Astronomy and the Center for Simulational Physics, University of Georgia, Athens, GA 30602-2451, USA.*

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Abstract. Total and state-selective charge transfer, ionization and stripping cross sections due to the collision of Si^{2+} ion with atomic hydrogen are investigated using the classical-trajectory Monte-Carlo (CTMC) method in the collision energy from 1 keV/amu to 10 MeV/amu. Total electron capture rate coefficient is obtained in the temperature range from 10^5 K^o to 10^8 K^o. Comparison with the data available shows that our CTMC results are reliable. The behaviors for these cross sections varying with the projectile energy are analyzed. A classical physical picture is presented to explain the reason behind the behaviors.

Key words: CTMC method; charge transfer; ionization; stripping.

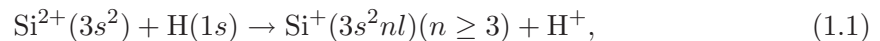
1 Introduction

Charge transfer, collisional ionization and stripping, as important processes of heavy particle collisions occur in astrophysics and laboratory plasma physics universally. Charge transfer is the dominant collision channel for ions with energies below about 0.1 MeV/amu, above which ionization is the most important channel. Charge transfer provides a recombination mechanism for multiply charged ions in *X*-ray ionized astronomical environments where there may be sparse electron and atomic hydrogen abundances (see, for example, Lepp and McCray [17]). In the divertor region of a tokamak fusion device, charge exchange

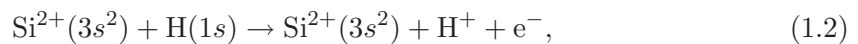
*Correspondence to: B. He, Key Laboratory of Computational Physics, Institute of Applied Physics and Computational Mathematics, Beijing 100088, P. R. China. Email: he_bin@mail.iapcm.ac.cn

of impurity ions with neutral atom and molecules plays an important role in the ionization balance and the production of radiative energy loss leading to cooling (Krasheninnikov et al. [15,16], Janev et al. [12]) and in the core of plasmas, charge exchange spectra produced by neutral beam injections is also an important method to diagnose the populations of stripping impurities. Recently, it is found these ion-atom/molecule charge transfer processes are of particular significance to EUV and X-ray emission from comets and from planetary atmospheres. Soft X-ray emissions have been observed from many comets, including comet Hale-Bopp (Owens et al. [23]) and comet Hyakutake (Lisse et al. [18], Mumma et al. [21]). It has been suggested that these X-ray emissions are due to charge transfer of heavy solar wind ions (such as O^{q+} , C^{q+} , Ne^{q+} and Si^{q+} , here $q = 1 - Z$ and Z is nuclear charge) with cometary neutral species such as H, O, H_2 , H_2O , OH and CO (Cravens [5], Haberli et al. [11]). Indeed, recent analysis of X-ray and EUV spectra of comet Hyakutake (Krasnopolsky and Mumma [14]) is said to have confirmed that such charge transfer processes are responsible for the observed X-ray emissions. In a similar way, X-ray emissions from the Jovian aurora are thought to be driven by charge transfer in collisions of multiply charged oxygen and sulfur ions with atmospheric neutrals such as H, He, and H_2 (Cravens et al. [6], Liu and Schultz [19]). Usually besides slow solar wind components, there exist fast solar wind components with the energies from 300 keV/amu to 3MeV/amu (Liu and Schultz [19]). The collision ionization of such fast charged ions with cometary neutral species or Jovian atmospheric neutrals is the most important way of their energy loss and becomes much more important than charge transfer. In the research of inertial confinement fusion (ICF), recent experiment shows the charge transfer may be important to explain some unusual high-intensity spectrum of silicon in the high-density and high-temperature plasmas (Elton et al. [8], Rosmej et al. [25]). In order to model and understand the behavior under these environments, it is necessary to obtain total and state-selective capture cross sections. Meanwhile, the ionization and stripping processes are the important competitive processes of electron capture. It is very necessary to include the ionization and stripping processes in the calculations because their cross sections are also needed in the simulations (Cravens et al. [6], Liu and Schultz [19]).

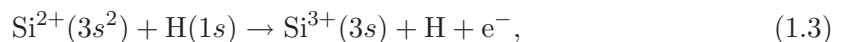
So far the collision processes of some charged ions such as O^{q+} , C^{q+} , N^{q+} with atomic hydrogen have been studied sufficiently in the analysis of X-ray and EUV spectra. However, there exist seldom data in the collisions of Si^{q+} ($q = 1 - 14$) with atomic hydrogen. In the previous paper, we investigated the collision processes of Si^{3+} with atomic hydrogen from 10^{-2} eV/amu to 10^6 eV/amu (Wang et al. [29]). In the present paper, we study the collision processes of Si^{2+} with H, namely, the charge transfer



the collision ionization



and the stripping process



using the classical-trajectory Monte-Carlo (CTMC) method in the projectile energy ranging from 1 keV/amu to 10 MeV/amu. Kim et al. [13] measured the total single-electron capture cross sections in the collision of Si^{2+} with H from 50 keV/amu to 200 keV/amu. Many years ago, McCarroll and Valiron [20] calculated the cross section and rate coefficient of charge transfer in the range of very low energy and temperature using quantal close-coupling method, and Gargaud et al. [9] at the same group calculated the charge transfer reaction rate from 10 K to 106 K with the similar method. Several years ago the total and state-selective charge transfer cross sections were calculated again by Clarke et al. [4] for energies less than 100eV/amu using a fully quantum-mechanical molecular-orbital close-coupling (MOCC) method, and the corresponding rate coefficients for the temperatures between 500 K^o and 10⁵ K^o were presented. In the same year, M.C. Bacchus-Montabonel obtained the cross section for charge transfer using a semi-classical approach in the energy range 0.1-1 keV /amu (Bacchus-Montabonel [3]). The *ab initio* potentials and couplings were used in the two later calculations, while a model potential molecular approach was used in McCarroll and Valiron [20] and Gargaud et al. [9]'s calculations. In general, the theoretical data available were only limited to the electron capture processes at low collision energy range (1 keV/amu). To our knowledge, there exist no theoretical data from intermediate to high projectile energies for the charge transfer process, and no experimental or theoretical results are available for the ionization and stripping processes. However, compared with the charge transfer, the ionization and stripping processes become more important in the higher projectile energy range.

It is well known that the CTMC method has been widely and successfully utilized to study the heavy-particle collisions over a wide projectile energy, in which all the competitive processes including charge transfer, collision excitation, ionization and stripping can be explicitly and simultaneously taken into account. In the present paper, the CTMC method is used to investigate the collisional process of Si^{2+} with H. Comprehensive comparisons with available experimental measurement and other theoretical data are performed, which indicate that our CTMC results are reasonable. The behaviors of these cross sections varying with the projectile energy are analyzed and a classical physical picture is presented to explain the reason behind the behaviors. Atom units are used throughout the paper unless stated otherwise.

2 Theoretical methods

In the present work, the CTMC method is utilized to calculate the charge-transfer, collisional ionization and stripping cross sections. As is well known, charge transfer is the dominant process in the collision of an charged ion with atom in the low projectile energy. But collisional ionization and excitation become important gradually with the energy increasing. When the projectile energy E_{proj} is beyond 10 keV/amu, these processes compete each other and it is difficult to deal with them simultaneously in the fully quantum-mechanical calculations. So far CTMC is a method widely used in the energy range, by

which reliable results can be usually obtained in a simple way. Although few quantum effects can be considered, especially for the active electron, the relevant cross sections thus obtained are usually in good agreement with experiment. There are some good introductions to the CTMC method (see Abrines and Percival [1], Olson and Salop [22], and here a brief description is given in the following.

The CTMC method simulates the ion-atom collision by sampling trajectories computed from a large ensemble of initial projectile-target configurations (see Abrines and Percival [1]). The collision processes are considered as a three-body problem, that is, the incident Si^{2+} ion, target nucleus H^+ and the active electron in target initially. The initial electronic orbits on the target are prepared in such a way as to mimic the quantum momentum distributions. The motion of the particles is then determined by an iterative solution of Hamilton's equations of motion. At the end of each Monte Carlo trajectory, the relative classical binding energies are calculated to judge if a reaction (charge transfer, ionization, elastic scattering, etc.) occurred. The final n, l -state after charge transfer, where n and l denote the principal and orbital quantum number respectively, can be determined assuming Bohr model and making a classical-quantum correspondence following the binning rules of Becker and MacKellar [2]. In the present paper the final projectile state for partially stripped ions is determined by the way suggested by Rakovic et al. [24],) where the quantum defect number μ_l for different l is employed. Here μ_l is calculated based on the ionization energies of the electrons obtained by Cowan code (see Cowan [7]). μ for s, p, d and f electron in Si^+ is found to be 1.37, 0.993, 0.254 and 0.061, respectively. All the μ_l for higher l than f are taken to be zero in our CTMC code.

In the collision of the partially stripped ion with H, the interaction of the ion with the electron initially resident on H is represented by a model potential describing the screening effect experienced by the electron as it approaches to the incident ion (see Garvey et al. [10]), which is expressed as

$$V(r) = -\frac{1}{r} \left(Z - (N - 1) \left[1 - \frac{1}{\eta/\xi(e^{\xi r} - 1) + 1} \right] \right), \quad (2.1)$$

where N is the electron number with the parameters η and ξ determined by fitting the numerical potential. This expression satisfies the asymptotic boundary conditions of Coulomb potential at infinite small and infinite large distances between the electron and the incident ion. For the projectile Si^{2+} , η and ξ are found to be equal to 1.102 and 3.26 respectively. If the target is multi-electronic atom or molecule, the similar screening model potential can be applied to the interaction between the electron and the target ion. In the present paper, the stripping process of $3s$ electron in Si^{2+} is also performed by CTMC method, where the potential for Si^{3+} in the form of Eq. (2.1) is used with $\eta = 1.489$ and $\xi = 3.479$ respectively. In this case the potential of atomic hydrogen is expressed as $(1.0 + 1/r)\exp(-2r)$, which is obtained by solving Poisson equation using the wave function of $1s$ electron in atomic hydrogen. As a relativistic invariant the total stripping cross section is calculated in the rest reference frame of Si^{2+} .

In our CTMC calculation at least 1 million trajectories are simulated for all the projectile energies and the corresponding maximum impact parameter is adjusted to ensure the results convergent and make statistical error as small as possible.

3 Results and discussions

3.1 Total and state-selective cross sections

Using CTMC method, ionization, stripping and charge transfer cross sections including total and state-selective single-electron capture in the collisions of Si^{2+} with H are calculated with E_{proj} from 1.0 keV/amu to 10 MeV/amu. The total cross sections are plotted in Fig. 1 with all the data available included. The statistical errors from CTMC method are usually about 1% of the corresponding cross sections, which could not be shown in the figures clearly.

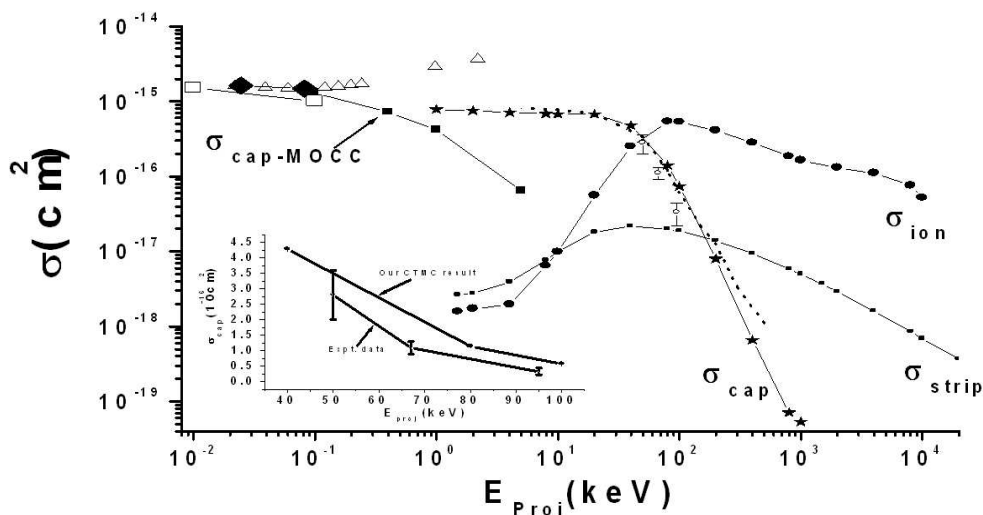


Figure 1: Total single-electron capture, ionization and stripping cross sections for $\text{Si}^{2+} + \text{H}$. Present CTMC result for charge transfer (line with filled stars), present CTMC result for ionization (line with full circles), CTMC result for capture with another potential (dotted line), present CTMC result for stripping (long line with full squares), present MOCC result for charge transfer (short line with full squares), Kim et al. [13] (open circles), M. C. Bacchus-Montabonel [3] (open triangles), Clarke et al. [4] (line with open squares), and Gargaud et al. [9] (full diamonds). In the inserted figure both the experimental data and our CTMC results for capture are shown in detail.

Using the potentials and couplings of Clarke et al. [4], we re-calculate the charge transfer processes $\text{Si}^{2+}(3s^2\ ^1S) + \text{H}(1s) \rightarrow \text{Si}^+(3s^23p\ ^2P) + \text{H}^+$ by the fully quantum-mechanical MOCC method (Wang et al. [26,27]), and get the same cross sections as Clarke et al. [4]'s in the energy range 0.01 - 100 eV/amu, which is not plotted in Fig. 1. We also extend our MOCC calculations in the energy range from 100 eV/amu to 1 keV/amu,

which are shown in Fig. 1 as the line with full squares. Usually the error bar is difficult to be given for MOCC results. There is about 10% deviation between our previous MOCC results (see Wang et al. [28]) and the experimental data near 1keV/amu. In the energy range $E_{proj} < 0.1$ keV/amu, the results of several MOCC calculations including Gargaud et al. [9] (full diamonds)'s, Clarke et al. [4]'s and Bacchus-Montabonel [3] (open triangles)'s are in excellent agreement with each other, and our MOCC results lie between Clarke et al. [4]'s and Bacchus-Montabonel [3]'s results. In the energy range from 0.1 keV/amu to 1 keV/amu, our MOCC cross sections becomes smaller with higher projectile energy and this behavior is reasonable because there exists only one avoided crossing point at internuclear distance of $12.84a_0$ in the potential curves of MOCC calculation (Clarke et al. [4]) and no higher energy levels than $\text{Si}^+(3s^23p^2\text{P})$ are included. However, Bacchus-Montabonel [3]'s cross sections increase slowly with increasing energy, and besides the radial couplings, Bacchus-Montabonel also included the rotational couplings. We think it is doubtful that the cross sections increase, not decrease, only because of the rotational couplings in the energy range 0.1-1 keV/amu. According to our previous work (Wang et al. [27], Turner et al. [30]), for the total charge transfer cross sections, the effect of rotational couplings is not important in the low energy rang ($E_{proj} < 1$ keV/amu). In addition to this, the CTMC results are usually higher than those from MOCC calculations and experiments since all the final different channels are included in CTMC calculation. But our present CTMC results are only about 1/3 of the maximum of M. C. Bacchus-Montabonel's [3] while they are still high above our MOCC results. In the energy range $E_{proj} > 0.1$ keV/amu, the interaction in a short internuclear distance ($< 2a_0$) may be important, and it is not easy to do the molecular-structure calculations in such a short distance, where there are so many avoided crossing points. Further MOCC calculation including the short-internuclear-distance interaction and more charge-transfer channels is needed to clarify this behavior.

Kim et al. [13] performed an experiment to measure the total capture cross sections in the high energy range and their data at three energies are displayed with open circles in Fig. 1. In order to make a clear comparison between the experimental data and our CTMC results, a small figure is inserted in the Fig. 1. Generally speaking, our results are in accordance with the experimental data. But looking at the inserted figure, it is found that the two experimental values near 70 keV/amu and 100 keV/amu are about 50% lower than our CTMC results although for the data close to 50keV/amu the discrepancy is smaller and ours lies in the range of the corresponding experimental error bar. For the difference we doubt whether it is because of the choice of the potential in our CTMC calculations. In order to check this point, another CTMC calculation of charge transfer is performed with a different potential. The potential is obtained by Hatree-Fock Slatter method (see Cowan [7]) and fitted as following:

$$V(r) = -\frac{2}{r} - \frac{12}{r}(1.0 + 0.5019r + 0.007436r^2) \exp(-2.3r). \quad (3.1)$$

However, no better agreement is found with this potential adopted, as shown with dotted

line in Fig. 1. Up to now, we can not explain the difference, and it may come from the errors in both of the experimental measurement and the CTMC calculations. Further experiments and theoretical calculations are needed to clarify it.

There exists a platform for the total electron capture cross section σ_{cap} with energies between 1 keV/amu and 10 keV/amu where charge transfer is the dominating inelastic process and the ionization cross section σ_{ion} rises up rapidly though it is much smaller than σ_{cap} . When $E_{proj} > 20$ keV/amu, σ_{cap} begins to decrease gradually and then drops quickly. With σ_{cap} decreasing, ionization becomes the dominant process gradually and σ_{cap} rises up rapidly to its maximum at about 100 keV/amu, which is about equal to the size of σ_{cap} in the platform. Beyond 100 keV/amu σ_{cap} begins to decline slowly. Compared with σ_{cap} and σ_{ion} , the stripping cross section σ_{strip} is always much smaller than the bigger one of them and it is always much insignificant. The main reason for this is that atomic hydrogen is neutral and must be very close to Si^{2+} so that there is strong enough interaction between H and the bound electron in Si^{2+} to ionize Si^{2+} . Besides this, the electron in 3s shell of Si^{2+} is much more tightly bound than that in H. Similar result for stripping could be found in the calculation by Liu and Schultz [19].

The state-selective single-electron capture cross sections are shown in Fig. 2. When $E_{proj} < 20$ keV/amu, the channel captured to $\text{Si}^+(3p)$ dominates all the other channels. This is consistent with our MOCC calculations in which only the channel captured to $\text{Si}^+(3p)$ is included. With the projectile energy increasing, the channels to higher energies become more and more important. When $E_{proj} > 20$ keV/amu, the channel captured to $\text{Si}^+(3d)$ dominates over others. By the simple calculation with Cowan's code, it could be found that among all the final states of charge transfer only the energy level of $\text{Si}^+(3p)$ is closest to that of $\text{H}(1s)$ (about 2.7eV lower). The energy levels of $\text{Si}^+(3d)$ and $\text{Si}^+(nl, n \geq 4)$ are at least 5.1eV higher than that of $\text{H}(1s)$. This is the reason that the channel to $\text{Si}^+(3p)$ is the most important one at low projectile energy. From the figure it also can be seen that both the state-selective cross sections for $\text{Si}^+(3p)$ and $\text{Si}^+(3d)$ decrease quickly when $E_{proj} > 30$ keV/amu. The cross sections to the higher excited states $\text{Si}^+(4l)$ are always much smaller than those to $\text{Si}^+(3l)$ until $E_{proj} > 70$ keV/amu. Beyond that energy, the capture to $\text{Si}^+(4l)$ could compete with that to $\text{Si}^+(3l)$ and can be ignored no longer. One fact worthy of note is that these cross sections captured to $\text{Si}^+(nl, n \geq 4)$ rapidly increase when $E_{proj} < 20$ keV/amu.

3.2 Classical picture of the collisional process

So far we have not seen an explanation for the behavior of the ionization and charge transfer cross sections including total and state-selective single-electron capture varying with the projectile energy. Here we try to make an explanation of the behavior using an classical physical picture. We think that at low projectile energy the electron mostly can be captured by the projectile directly because the energy levels of the final states for charge transfer are close to that of $\text{H}(1s)$. Besides this, although the electron may become free tentatively during the collisional process, it usually owes with small velocity so that

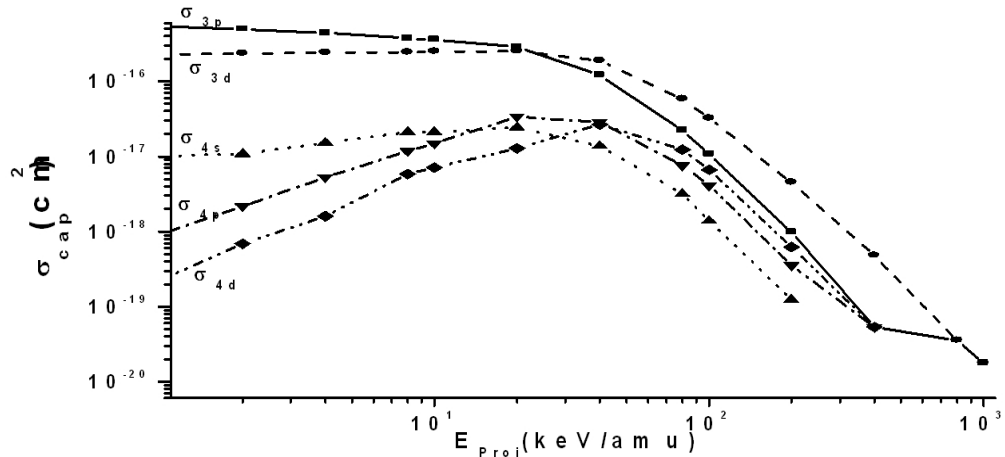


Figure 2: State-selective single-electron capture cross sections for different final states of Si^+ .

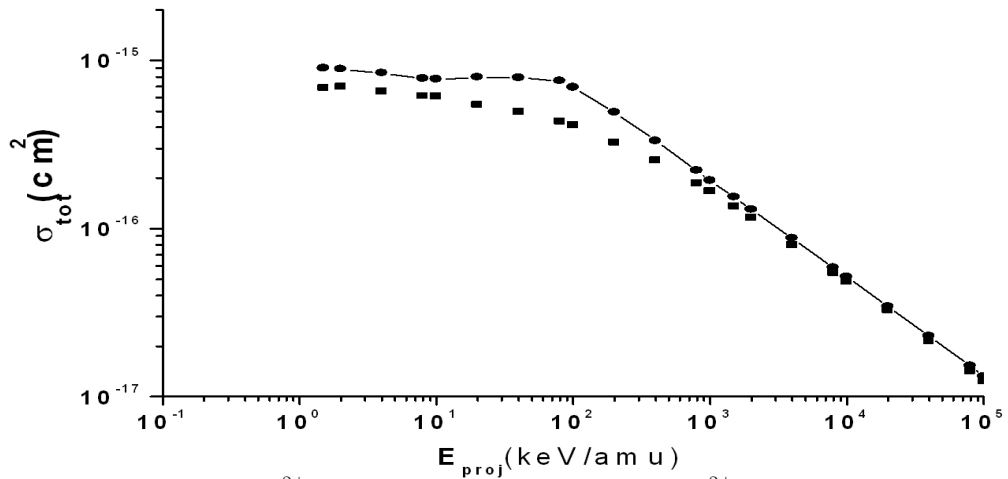


Figure 3: $\sigma_{cap} + \sigma_{ion}$ for $\text{Si}^{2+} + \text{H}$ (full squares) and σ_{ion} for $\text{anti-Si}^{2+} + \text{H}$ (line with full circles).

it could move with the projectile and become captured at last. In this way the charge transfer is the dominant process at such a energy. With E_{proj} increasing gradually, the projectile moves faster. Then only the tentatively ejected electrons with a higher velocity can move with the projectile and be captured finally, which leads to the decreasing of the capture cross section and the increasing of the ionization cross section. In this way more electrons moves a little slower than the projectile during the projectile leaves the target. This results in the increasing of the average kinetic energy of the electrons relative to the projectile. That means that more electrons are captured to higher excited states of the projectile and the selective cross sections to these states rise up. With further increasing of E_{proj} , less and less electrons are ejected with almost the same velocity of the projectile so that charge transfer turns insignificant rapidly and ionization becomes the much more important process. In addition to the above mentioned reason the electrons, which are directly captured by the projectile and be free no longer, usually become less and less with

increasing projectile velocity or energy. With much higher projectile energy, the projectile moves very fast and the time of the interaction between the projectile and target becomes very short. So the bound electron of the target can not get a strong enough impulse to be free unless the projectile is very close to the target, which leads to the rapid reduction of the ionization cross section. Our view can be verified in Fig. 3.1, which gives the changing of the ionization cross section with E_{proj} where the projectile is an fictitious anti-particle of Si^{2+} (anti- Si^{2+}). For the kind of the fictitious projectile only charge transfer is forbidden. In the figure the total cross section for the projectile Si^{2+} , which is the summation of the total charge transfer and ionization cross section, is also shown with full squares. Comparison of the two kinds of results indicates that they are close when $E_{proj} < 100$ keV/amu. This means that most of the electrons, which could be ionized in the collision of anti- Si^{2+} with atomic hydrogen, become captured in the collision of Si^{2+} with atomic hydrogen when E_{proj} is small, which causes that charge transfer is much important than ionization in the projectile range. It also can be found that with E_{proj} increasing the two curves gradually become almost the same one, which means that in this case less and less electrons can be captured and gradually ionization becomes more and more important than charge transfer. From the above discussion we know that in charge transfer some electrons may become free to both the projectile and target simultaneously at some time and finally are captured by the projectile. Fig. 4 gives the ratio of such electrons to the whole ones in charge transfer varying with the projectile energy. From the figure it can be seen that generally speaking, more and more electrons which are finally captured become free at one time or another as E_{proj} increases.

As further description of the above physical picture, one CTMC trajectory is potted in Fig. 5 at 10 keV/amu. The trajectory shows the history of single electron capture process. At beginning, the electron is far from the incident ion and the electron energy relative to the incident ion E_{ep} is approximately 0.2 a.u.; that relative to the target nucleus E_{et} keeps negative and the distance between the electron and the target ion displays an oscillating behavior. With the time evolution, the projectile approaches to the electron gradually and E_{ep} changes violently. When the projectile is very close to the electron, the electron becomes captured by the projectile. But with the influence of the target nucleus the electron is not captured by the projectile at all times. Sometimes it may be captured simultaneously by both the projectile and the target nucleus, sometimes it become completely free with both E_{ep} and E_{et} being positive. When both the electron and the projectile are gradually far away from the target nucleus, which influence to the electron becomes more and more weaker, the electron becomes captured completely by the projectile with E_{ep} keeping negative while their relative distance R_{ep} oscillates in a certain range.

3.3 Total charge transfer rate coefficient

In order to apply for astrophysics and fusion plasmas conveniently, the total electron-capture rate coefficients are calculated using our MOCC data at low projectile energies

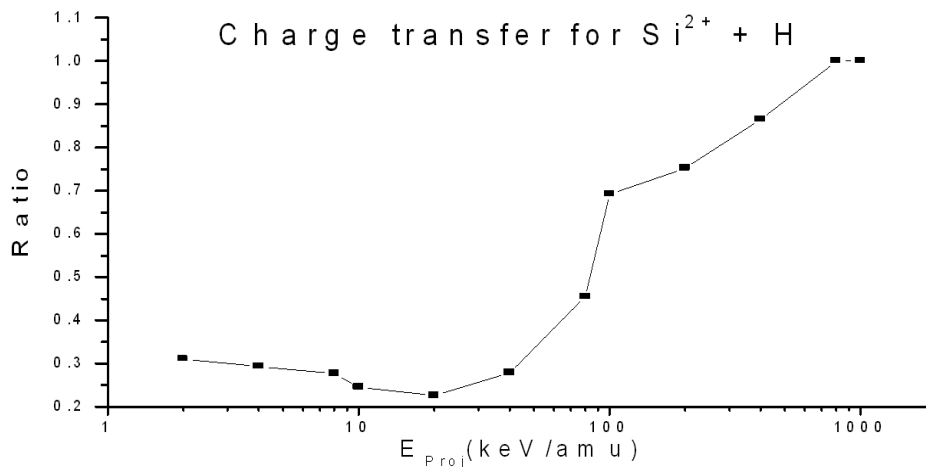


Figure 4: Ratio of the events with the electrons which are free at some time to the total events for charge transfer process.

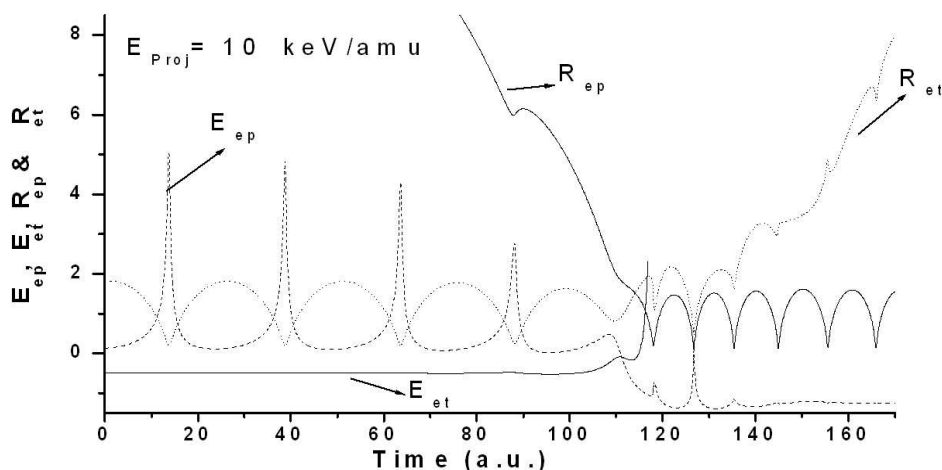


Figure 5: One CTMC trajectory at 10 keV/amu as a function of time. Electron energy relative to the target nucleus E_{et} (solid line) and to the projectile E_{ep} (dashed line), distance between electron and the projectile R_{ep} (solid line) and between electron and the target nucleus R_{et} (dotted line).

and CTMC data from intermediate to high energies. The results in the temperature range from 10^5 K $^\circ$ to 10^8 K $^\circ$ are plotted in Fig. 6. The rate coefficients at lower temperature, which have been given precisely by Clarke et al. [4], are displayed here no longer. The results of Gargaud et al. [9] are also plotted in the figure with scattering points, which are about 50% higher than ours. The reason may come from the different potentials and avoided crossing points in MOCC calculations, as has been pointed out by Clarke et al. [4].

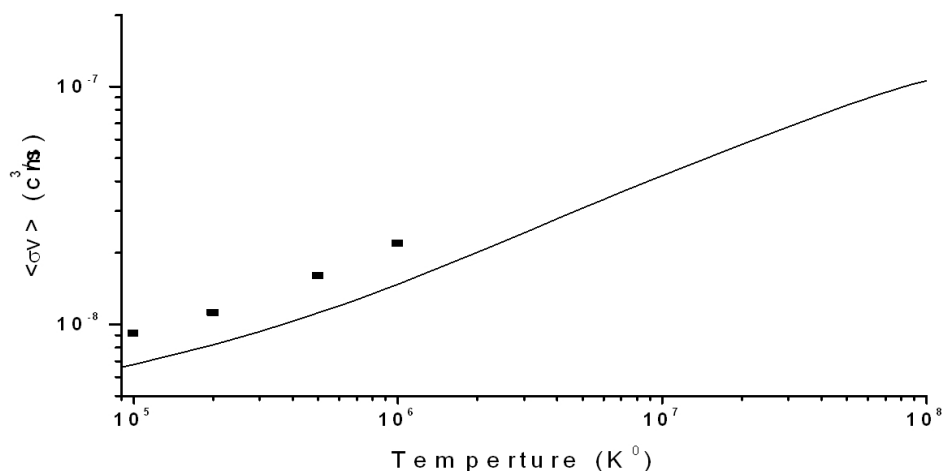


Figure 6: Total single-electron capture rate coefficient. Present result (line), Gargaud et al. [9] (full square).

4 Summary

Total and state-selective charge transfer, ionization and stripping cross sections due to the collision of Si^{2+} ion with atomic hydrogen have been calculated using the CTMC method in the energy range from 1 keV/amu to 10 MeV/amu. Total electron capture rate coefficient is also calculated in the temperature range from 10^5 K^0 to 10^8 K^0 . Comparison with the data available shows that our CTMC results are reasonable. The behaviors for these cross sections varying with the projectile energy are analyzed and explained with a classical physical picture. It is found that the electrons, which could be ionized in the collision of anti-particle with atomic hydrogen, become captured in the collision of ion with atomic hydrogen when the projectile energy is small. This causes that charge transfer is much important than ionization for low projectile energy. As the projectile moves faster, only those electrons with higher velocity in the collision can move with the projectile and be captured finally. This leads to the decreasing of the capture cross section and the increasing of the ionization cross section. In this way collisional ionization gradually becomes much more important than charge transfer. When the projectile energy is very high, the time of the interaction between the projectile and target becomes very short which results in rapid reducing of the ionization cross section.

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