Charge-transfer cross sections of H^+ ions in collisions with Ne atoms in the energy range below 4.0 keV

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Total charge-transfer cross sections for H^+ ions in collisions with Ne atoms have been measured in the energy range of 0.60 to 3.6 keV with the initial growth rate method and found to agree with the present rigorous calculation based on a molecular-orbital expansion method with the electronic states obtained by the multireference single- and double-excitation configuration interaction method. These observed cross sections are also compared with previously published data and theoretical prediction. It has been found that previous experimental data deviate significantly from the present observed and calculated cross sections as the collision energy decreases.

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I. INTRODUCTION

Charge transfer of low energy H^+ ions (protons) colliding with noble gas atoms (He, Ne, and Ar) is important as one of the most fundamental atomic collision processes as well as in various applications. For example, these collisions play a key role in cooling and diagnostics of low temperature edge plasmas in the current controlled thermonuclear fusion devices with a gas puffing system [1,2].

There have been extensive experimental investigations of such processes. Earlier studies performed before 1958 and their data involving hydrogen atoms, helium ions, and atoms at kinetic energies above 0.2 keV were compiled and assessed in a review article of Allison [3]. Later, another review article was presented by Tawara and Russek [4] and the compiled data by Tawara [5] were published. At collision energies below 10 keV, experimental data by Stedeford and Hasted [6], Williams and Dunbar [7], and Rudd *et al.* [8] were available for H^++Ne collisions. Since these data sets were found to be closely consistent with each other, it was believed so far that the cross section data for charge transfer in this collision system were well established and understood.

On the other hand, theoretical approaches applicable to slow ion collisions involving multielectron targets are limited and scarce. Kimura and Lane have developed and summarized a molecular-orbital close-coupling method (MOCC) in order to calculate the partial as well as total charge transfer cross sections of low energy ions colliding with various atoms and molecules [9] and indeed have shown that this method can reproduce well the observed partial ($2s$ and $2p$) cross sections in H^++Ne collisions over 1–10 keV [10]. Another approach, the nonperturbative basis generator method (BGM) with the optimized potential method (OPM), has been applied to H^++Ne collisions in the 1 keV–5 MeV regions by Kirchner, Lüdde, and Dreizler [11]. Their calculated total charge-transfer cross sections were in excellent accordance with the earlier experimental data at energies above 5 keV. They also presented the partial cross sections for capture into the K ($n=1$) and the L ($n=2$) shells of H atoms in the energy range of 1.0 to 30 keV. The BGM-OPG cross sections for capture into the L shell are in good accord with the experimental data of Tepehan *et al.* [10] and of Hippler *et al.* [12]. However, the total cross sections obtained with the BGM-OPG method which were determined by summing up the partial capture cross sections into specific shells were found to decrease steeply in contrast to the previous experimental results below 5 keV as the collision energy decreases [13]. Indeed, it has been found that their calculated results at 1 keV are smaller by a factor of 8 than the experimental cross section. Also, during the course of theoretical investigations on laser-assisted ion collisions [14], it was noticed that there seems to be some serious inconsistency in old data for electron capture in low-energy proton collisions. Therefore, we have concluded that it is necessary to resolve this discrepancy.

To obtain precise and reliable cross section data and a detailed understanding of the collision dynamics, therefore, we have carried out a joint experimental and theoretical study for charge transfer of H^+ ions colliding with Ne atoms at low keV energies. In the present experiment, the total cross sections of charge transfer in this collision have been determined in the energy range of 0.60 to 3.6 keV by applying an initial growth rate method. In the present theoretical calculation, the (MOCC) method is applied to this specific process. The observed cross sections are compared with the

present calculations and other previously published theoretical results.

II. EXPERIMENTAL METHOD

A detailed description of the present experimental apparatus and methods has been previously given [15,16], and so only some essential features will be briefly mentioned here.

A mass-analyzed H^+ ion beam produced from an electron impact ion source penetrated through a collision cell filled with the target neon gas of high purity (>99.95%). The primary H^+ ions and product neutral H atoms emerging from the cell after charge-transfer collisions were charge-separated with an electrostatic deflector and detected with a position-sensitive microchannel plate detector (MCP-PSD). From the integrated counts of each peak corresponding to H^+ ions and H atoms recorded on a pulse height analyzer as a position-charge spectrum, the fraction F_0 of neutral hydrogen atoms was derived as a function of the target gas pressure (or target thickness). The charge-transfer cross sections were determined from the slope of the linear part of the observed fraction curve F_0 (growth rate method), after confirming that the detection efficiencies of the present MCP-PSD for H^+ and H particles were identical within the experimental uncertainties over the present collision energy range (see Ref. [17] in more detail).

The statistical uncertainties of the cross sections were within 6% in the energy range above 0.80 keV and 33.7% at 0.60 keV. Systematic uncertainties due to the determination of the target thickness, the temperature of target gases, and so forth are estimated to be from 9.76 to 14.7% for determining the absolute cross sections. Total experimental uncertainties of the absolute cross sections are given as the quadratic sum of these uncertainties involved.

III. THEORETICAL METHOD

A. Molecular states

The adiabatic potential curves and molecular wave functions of the NeH^+ system are obtained by employing the *ab initio* multireference single- and double-excitation configuration interaction (MRD-CI) method [18] with configuration selection at a threshold of 1.0×10^{-7} hartrees and energy extrapolation, using the Table CI algorithm [19]. In the present CI calculation, the two electrons in the first (lowest) molecular orbital (MO) are kept inactive, while the highest MO is discarded. The radial coupling matrix elements are calculated with the resulting CI wave functions by employing a finite-difference method [20], while the corresponding rotational matrix elements are computed analytically. The cc-pVQZ (correlation-consistent polarization valence quadruple zeta) basis set [21] has been used in the calculation for the Ne atom, but its g function is discarded. In addition, several diffuse functions have been added. The basis set for the neon atom is thus (14s, 8p, 3d, 2f) contracted to [7s, 6p, 3d, 2f]. A conventional basis set for the hydrogen atom is employed, and this has been augmented with a single d-type function of exponent 0.5.

TABLE I. Observed and calculated cross sections (in units of 10^{-17} cm^2) of charge transfer by H^+ ions from Ne atoms.

H^+ energy (keV)	Observed cross section	Calculated cross section
0.60	0.235±0.087	0.102
0.80	0.639±0.092	0.338
1.0		0.604
1.2	1.67±0.19	1.73
1.8	3.31±0.34	4.74
2.0		5.89
2.5	6.69±0.66	9.04
3.0		13.3
3.6	14.1±1.4	16.4
4.0		19.8
6.0		27.1
8.0		30.2
10		30.4
20		25.2

B. Scattering dynamics

The molecular-orbital close-coupling (MOCC) method within the semiclassical impact parameter formalism [9] has been employed, that is, the relative motion of the projectile nucleus is treated classically with a straight-line trajectory and the electronic motion is treated quantum mechanically. The total wave function of this collision system is expanded in terms of products of molecular states and electron translation factors (ETFs). The ETF ensures that the asymptotic scattering conditions are satisfied. Substituting the total wave function into the time-dependent Schrödinger equation, we obtain coupled equations as a function of time. All radial and rotational coupling matrix elements among molecular states considered are included in the present calculations. The transition amplitudes can be obtained by solving the coupled equations and the cross sections are then determined by integration of the square of these quantities over the impact parameter.

We have employed a basis set including the initial $[Ne(^1S)+H^+]$ and the final $[Ne^+(^2P)+H\ (n=1,2,3)]$ states, in addition to some of the target excited $[Ne^*(3s,3p)+H^+]$ states.

IV. RESULTS AND DISCUSSION

The present experimental and calculated total cross sections for charge transfer of H^+ ions from Ne atoms are given in Table I, and are also shown in Fig. 1 together with the previously published experimental data and theoretical prediction.

It is apparent that the present experimental charge-transfer cross sections decrease very steeply as the collision energy decreases. This behavior is expected to occur at low collision energies for the present collision system that has a large energy defect between the initial and charge-transferred chan-

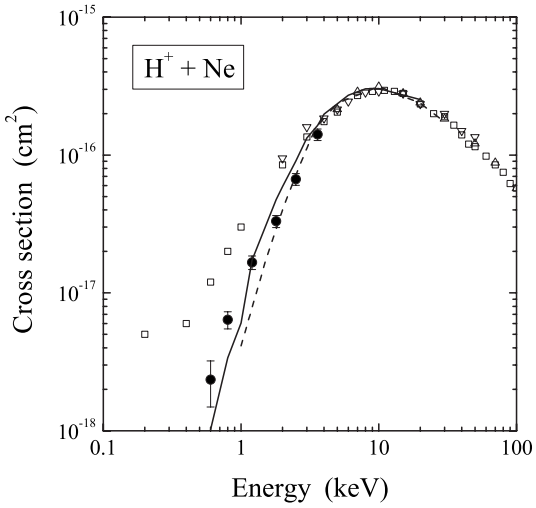

FIG. 1. Total charge-transfer cross sections of H^+ ions colliding with Ne atoms. Experiment: ●, present data; □, the evaluated value by Allison [3] (based primarily on data by Stedeford and Hasted [6]); ▽, Williams and Dunbar [7]; △, Rudd *et al.* [8]. Theory: —, present MOCC calculation;-----, Kirchner, Lüdde, and Dreizler [11].

nels. The deviation observed between the present results and those of Stedeford and Hasted [6] is found to become more significant as the collision energy decreases. In fact, their data are found to be larger by a factor of about 5 at 0.6 keV and about 3 at 0.8 keV, respectively, than the present observed cross sections. The total cross sections calculated by Kirchner, Lüdde, and Dreizler [11] based on the BGM-OPG method are in general accordance with the present measurements at energies above 2 keV, but become gradually smaller than the present experimental results below 2 keV. The present MOCC calculations are found to reproduce well the BGM-OPG calculations in the entire energy region studied, but it is also found that the BGM-OPG calculated values are smaller than the present MOCC results by about 30% below 2 keV. The present MOCC calculations are generally in accordance with the present measurements. In the energy range above 1.5 keV, however, the present experimental values are smaller than the present calculated results, and the situation is reversed below 1.2 keV. Though it is not possible to single out any particular reason for this deviation, we believe that the accumulated error for small contributions from both experiment and theory are most likely responsible.

In conclusion, the present experimental and theoretical joint work has provided reasonably reliable cross sections for the charge transfer of the Ne/H^+ system at low energies. It also should be pointed out that it would also be important to determine the cross sections at still lower energies.

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[1] R. K. Janev, *Atomic and Molecular Processes in Fusion Edge Plasmas*, edited by R. K. Janev (Plenum, New York, 1995), p. 1.
[2] *ITER Physics Basis*, edited by D. W. Ignat [Nucl. Fusion **39**, 2417 (1999)].
[3] S. K. Allison, Rev. Mod. Phys. **30**, 1137 (1958).
[4] H. Tawara and A. Russek, Rev. Mod. Phys. **45**, 178 (1973).
[5] H. Tawara, At. Data Nucl. Data Tables **22**, 491 (1978).
[6] J. B. H. Stedeford and F. B. Hasted, Proc. R. Soc. London, Ser. A **227**, 466 (1955).
[7] J. F. Williams and D. N. F. Dunbar, Phys. Rev. **149**, 62 (1966).
[8] M. E. Rudd, R. D. DuBois, L. H. Toburen, C. A. Ratcliffe, and T. V. Goffe, Phys. Rev. A **28**, 3244 (1983).
[9] M. Kimura and N. F. Lane, in *Advances for Atomic, Molecular and Optical Physics*, edited by D. R. Bates and B. Bederson (Academic, New York, 1989), Vol. 26, p. 76.
[10] G. G. Tepehan, B. Siegmann, H. Madeheim, R. Hippler, and M. Kimura, J. Phys. B **27**, 5527 (1994).
[11] T. Kirchner, H. J. Lüdde, and R. M. Dreizler, Phys. Rev. A **61**, 012705 (1999).
[12] R. Hippler, W. Harbich, H. Madeheim, H. Kleinpoppen, and H. O. Lutz, Phys. Rev. A **35**, 3139 (1987).
[13] T. Kirchner (private communication).
[14] T. Kirchner, Phys. Rev. Lett. **89**, 093203 (2002).
[15] T. Kusakabe, H. Yoneda, Y. Mizumoto, and K. Katsurayama, J. Phys. Soc. Jpn. **59**, 1987 (1990).
[16] T. Kusakabe, K. Asahina, J. P. Gu, G. Hirsch, R. J. Buenker, M. Kimura, H. Tawara, and Y. Nakai, Phys. Rev. A **62**, 062714 (2000).
[17] T. Kusakabe, M. Kimura, L. Pichl, R. J. Buenker, and H. Tawara, Phys. Rev. A **68**, 050701(R) (2003); T. Kusakabe, Y. Miyamoto, M. Kimura, and H. Tawara, *ibid.* **73**, 022706 (2006).
[18] R. J. Buenker and S. D. Peyerimhoff, Theor. Chim. Acta **35**, 33 (1974); **39**, 217 (1975); R. J. Buenker, Int. J. Quantum Chem. **29**, 435 (1986); S. Krebs and R. J. Buenker, J. Chem. Phys. **103**, 5613 (1995).
[19] R. J. Buenker, in *Proceedings of the Workshop on Quantum Chemistry and Molecular Physics*, Wollongong, Australia, edited by P. G. Burton (University Press, Wollongong, 1980); in *Studies in Physical and Theoretical Chemistry*, edited by R. Carbo, Current Aspects of Quantum Chemistry (Elsevier, Amsterdam, 1981), Vol. 21, p. 17.
[20] G. Hirsch, P. J. Bruna, R. J. Buenker, and S. D. Peyerimhoff, Chem. Phys. **45**, 335 (1980).
[21] T. H. Dunning, Jr., J. Chem. Phys. **90**, 1007 (1989).