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Low-energy charge transfer for collisions of Si^{3+} with atomic hydrogen

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Cross sections of charge transfer for Si^{3+} ions with atomic hydrogen at collision energies of ≈40–2500 eV/u were carried out using a merged-beam technique at the Multicharged Ion Research Facility at Oak Ridge National Laboratory. The data span an energy range in which both molecular orbital close coupling (MOCC) and classical trajectory Monte Carlo (CTMC) calculations are available. The influence of quantum mechanical effects of the ionic core as predicted by MOCC is clearly seen in our results. However, discrepancies between our experiment and MOCC results toward higher collision energies are observed. At energies above 1000 eV/u good agreement is found with CTMC results.

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I. INTRODUCTION

Charge transfer (also called charge exchange or electron capture) of positively charged ions with atomic hydrogen is important in magnetically confined plasmas where interactions at the edge of the plasma between impurity ions and H atoms from the chamber walls influences the overall ionization balance and affects the plasma cooling [1,2]. In astrophysics, charge transfer plays a role in determining the properties of the observed gas [3,4]. The charge transfer process studied in this work,

$$Si^{3+} + H(1s) \rightarrow Si^{2+} + H^{+}, \qquad (1)$$

is an important destruction mechanism of Si^{3+} in photoionized gas [3]. Furthermore, soft x-ray emission from comets has been explained by charge transfer of solar wind ions, among them Si^{3+}, with neutrals in the cometary gas vapor [5].

Recently, Wang *et al.* [6] published cross sections for charge transfer of Si^{3+} with atomic hydrogen obtained using two different theoretical methods: the classical trajectory Monte Carlo (CTMC) method and the molecular orbital close coupling (MOCC) method. The CTMC method uses an ensemble of electron orbits chosen to mimic the quantum mechanical initial state and treats the ion-atom collision by solving the classical mechanical equation of motion for the projectile ion, target atomic core, and active electron, in order to determine the reaction cross section. This model is expected to be accurate toward high collision energies where quantum effects can be neglected. At lower collision energies, the relative nuclear motion between the collision partners is slow compared to the orbital motion of the active electrons in the system. Thus, electrons of the temporary quasimolecule formed in the collision have sufficient time to adjust to the changing interatomic field as the nuclei approach and separate. Cross sections can also be very dependent on the number of electrons in the ion core. The MOCC approach is considered most accurate at these energies but is difficult to perform. The MOCC method solves the time-dependent Schrödinger equation for all particles in the collision in an expansion describing the dominant scattering channels involved in the collision in terms of basis functions of the projectile-target molecular states.

Previous experimental studies of the Si^{3+}+H system, performed using a fast ion beam and a static atomic hydrogen oven as a target, were limited to collision energies above about 50 keV/u [7]. At these energetic collisions, many states are involved and the individual quantal nature of states is washed out. Not surprisingly, CTMC predictions compare well with the high-energy measurements [7].

In the present work, we performed absolute cross section measurements of reaction (1) in the energy range between 44 and 2444 eV/u using the upgraded ion-atom merged-beam apparatus [8] at the Multiply Charged Ion Research Facility (MIRF) at Oak Ridge National Laboratory (ORNL). The data span an energy range in which both the MOCC and CTMC calculations are available. The rest of this paper is organized as follows: In Sec. II, we briefly describe the experimental apparatus. In Sec. III we discuss our results and compare with the available theories. Finally, a summary is presented in Sec. IV.

II. EXPERIMENTAL PROCEDURE

An in-depth description of the ion-atom merged-beam technique at the Multiply Charged Ion Research Facility is given in [9,10]. The ion-atom merged-beams apparatus has been upgraded [8,11] to accept higher-velocity beams from a 250 kV High Voltage Platform at MIRF. In the present experiment, beams of ground state atomic hydrogen at 8 and 9 keV kinetic energy were merged with a beam of Si^{3+} ions

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extracted from a permanent magnet electron cyclotron resonance (ECR) source. The kinetic energy of the Si ions was varied from 56 to 215 keV in order to vary the center-of-mass collision energy $E_{\text{c.m.}}$, between the ions and H. At all energies the Si^{3+} current was about 5 μA. The 20 nA particle current of atomic hydrogen was produced by tuning a beam of H^- ions, created in a duoplasmatron source, through a neodymium-doped yttrium aluminum garnet (Nd:YAG) laser cavity, where some of the H^- ions were neutralized through photodetachment, leaving the kinetic energy of the hydrogen atoms unchanged. The H^- parent beam was then electrostatically deflected out of the atomic hydrogen beam. The atomic H beam passed through a hole in the outer electrode of a 65° electrostatic spherical deflector that bent the Si^{3+} ion beam to run collinear and overlap with the neutral beam. Protons created from the charge transfer reaction (1) in the merge path as well as the parent and daughter silicon beams were magnetically dispersed from the hydrogen beam at the end of the merge path. The silicon ions of both charge states (parent and product ions) were collected by the same Faraday cup. The neutral H parent beam struck a stainless steel surface, where the measured secondary electron emission current allowed us to determine the H particle current through the secondary electron emission yield $\gamma = 1.54 \pm 0.08$. The measurement of γ was performed *in situ* [9] before and after the beam time. The charge transfer product protons were additionally bent out of the magnetic analyzer plane by an electrostatic deflector and then detected by a channeltron in single-particle counting mode. The beam-beam signal (Hz) was separated from backgrounds (kHz) using a beam-modulation technique [9].

While photodetachment of H^- produces a H beam in the ground state, collisional stripping of the H^- parent ions on rest gas leads to small impurities of hydrogen atoms in highly excited electronic states that can have orders of magnitude higher cross sections for charge transfer than ground state hydrogen atoms. These excited state atoms in the neutral beam can falsify the measured beam-beam signal rate despite their sparseness. In order to reduce their contribution to the measured signal, the neutral beam passed through a field ionizer with a field strength of 30 kV/cm that either quenches or strips (down to about $n = 12$) the neutrals in excited states [12,13]. The remaining excited atom contribution to the measured signal is determined and corrected for by repeating the charge transfer cross section measurements with the photodetachment laser switched off, i.e., with neutrals produced solely through collisional stripping on rest gas. Typically, this easily quantified correction to the signal is smaller than 5%.

Below 44 eV/u the signal-to-background ratio was insufficient to collect statistically significant data. This was due, in part, to a small cross section and a relatively weak Si^{3+} beam compared to other merged-beam measurements, which extend down to meV/u energies [10]. Thus we were unable to collect data at lower energies since, even if the cross section did increase as $1/v$ as predicted for collision energies $E_{\text{c.m.}} < 5$ eV/u, the signal rate would not increase since the rate $R \propto \sigma v$ would be constant with decreasing $E_{\text{c.m.}}$.

A detailed, comprehensive systematic error analysis is given in [9]. An important systematic uncertainty originates from the beam-beam overlap measurements performed before and after taking data for each data point. Recently, we have significantly improved the overlap determination system by means of a rotating dual-wire scanner [14]. Together with the other systematic error sources [9], we estimate the systematic contribution to our total uncertainty to be 12% at a 90% confidence level.

TABLE I. Cross sections measured with two different H beam energies are listed below. Statistical and total uncertainties are given at the 90% confidence level. See text for details.

H beam energy (keV)	Collision energy (eV/u)	Cross section (10^{-16} cm^2)	Uncertainties Statistical (10^{-16} cm^2)	 Total (10^{-16} cm^2)
9	44	1.17	0.45	0.47
9	86	1.99	0.67	0.72
9	139	3.58	0.66	0.79
9	236	5.05	0.44	0.75
9	320	7.46	0.58	1.06
9	412	7.70	0.39	1.00
9	459	7.21	0.58	1.04
9	622	10.23	0.38	1.28
9	850	11.32	0.51	1.45
8	858	10.70	0.79	1.49
9	952	14.79	0.46	1.83
9	1061	14.76	0.41	1.81
9	1180	16.68	0.38	2.03
9	1449	16.90	0.55	2.10
8	1460	15.83	0.70	2.02
8	1764	16.59	0.86	2.17
9	1908	14.88	0.32	1.81
8	2051	14.96	1.32	2.23
9	2444	15.53	0.95	2.09

III. RESULTS AND DISCUSSION

The data obtained in this work are shown in Table I. In Fig. 1, we compare our results with the theoretical predictions found using the MOCC and CTMC methods, both described in [6]. The CTMC calculations have since been extended toward lower energies [15] for comparison with our experimental results. Although our experimental work covered a different energy range from the one performed by Kim *et al.* [7], their experimental data are also shown in Fig. 1 for completeness. The measurements using an 8 keV H beam were performed in a second beam time two months after the 9 keV run in order to verify the transition from increasing cross section to the high-energy plateau at around $E_{\text{c.m.}} \approx 1200$ eV/u.

CTMC calculations can yield reliable results at high collision energies where many states are involved and individual states' contributions to the cross section are averaged out. Being a classical model, the CTMC can fail at lower center-of-mass energies, where fewer states are active and

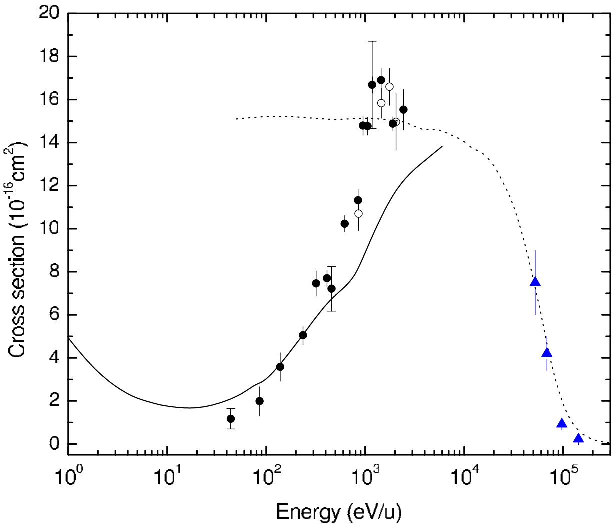

FIG. 1. (Color online) Comparison of the present experimental results with theory. Solid line, MOCC calculations [6]; dashed line, CTMC results [6] recalculated including lower collision energies [15]; full and open circles, this work (two separate beam times) with statistical errors at a 90% confidence level. Error bars with horizontal dashes show the total uncertainty including the estimated 12% relative systematic error added in quadrature. Full triangles, results of Kim *et al.* [7].

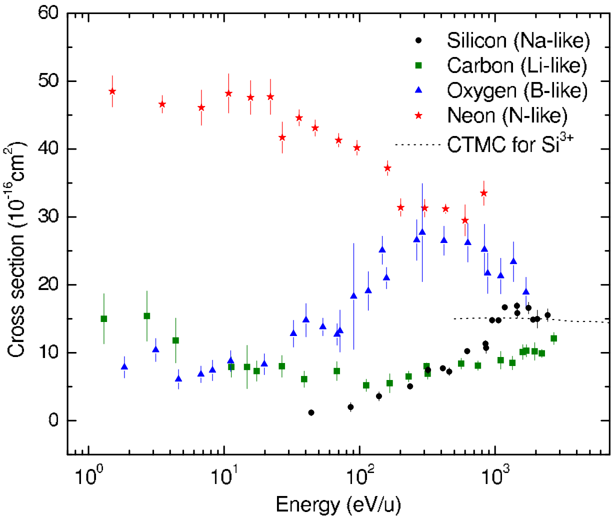

FIG. 2. (Color online) Cross section for charge transfer of hydrogen with different ions with charge $q=+3$, all shown with statistical errors at a 90% confidence level. Full circles, this work; dashed line [6,15]; squares [19]; triangles [20]; and stars [21].

quantum mechanical effects like couplings between states and dynamical effects become dominant. If couplings, e.g., with the core electrons, favor some reaction channels and suppress others, MOCC calculations are appropriate. To illustrate this, we show in Fig. 2 a comparison of the charge transfer cross section for different ions with charge +3, all obtained using the ORNL ion-atom merged-beam apparatus. It is obvious from the figure that the number of core electrons on the ion plays an important role for the charge transfer process toward lower energies. At 50 eV/u, there is more than a factor of 5 difference in the cross sections for Si^{3+} and Ne^{3+}. At higher energies, the cross sections for the reactions with different ions of the same charge state appear to converge to the CTMC value. Note that this value is different by a factor of 2 from the experimental scaling of [16] ($\sigma=q\times10^{-15}$ cm^2), which is thought to be applicable to charge transfer with atomic H for ions with cores that have (at least) a few bound electrons.

As seen in Fig. 1, our measurements for Si^{3+} confirm the trend predicted by MOCC calculations. However, we find a faster rise of the cross section with increasing collision energies, and above $E_{\mathrm{c.m.}}\approx1000$ eV/u find good agreement with the plateau predicted by the CTMC method. The MOCC results, however, suggest that the CTMC data are reliable only above $E_{\mathrm{c.m.}}=6000$ eV/u. The MOCC data may underestimate the cross section at the highest energies due to the limited basis used in the calculation [17]. Also, Wang *et al.* [6] emphasize that their MOCC calculation does not include electron translation factors [18] that are expected to become important for $E_{\mathrm{c.m.}}\geq1000-5000$ eV/u. Below $E_{\mathrm{c.m.}}\approx1000$ eV/u, it is evident that the limit of the classical CTMC method seems to be reached, for we see the drop in the measured cross section that indicates the rising importance of quantum effects toward lower collision energies. Below $E_{\mathrm{c.m.}}=460$ eV/u, the MOCC results agree well with our experimental data. Our lowest collision energy data point at $E_{\mathrm{c.m.}}=44$ eV/u seems to lie just below the predicted cross section, but given our experimental uncertainty the agreement is still satisfactory.

IV. SUMMARY

Using a merged-beam approach we have measured the cross section for charge transfer for Si^{3+} ions with ground state atomic hydrogen for the collision energy range of $E_{\mathrm{c.m.}}\approx40-2500$ eV/u. Our results show that the classical CTMC model gives a reliable prediction above $E_{\mathrm{c.m.}}\approx1000$ eV/u. The more sophisticated MOCC method is in good agreement with our experiment for collision energies lower than $E_{\mathrm{c.m.}}=460$ eV/u. It remains an open question if the effects not included in the MOCC calculation by Wang *et al.* [6] will resolve the disagreement with our data above $E_{\mathrm{c.m.}}=460$ eV/u.

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[1] S. I. Krasheninnikov, A. Yu. Pigarov, and D. J. Sigmar, Phys. Lett. A **214**, 285 (1996); A. Yu. Pigarov and S. I. Krasheninnikov, *ibid.* **222**, 251 (1996).

[2] R. K. Janev, T. Kato, and J. G. Wang, Phys. Plasmas **7**, 4364 (2000).

[3] J. B. Kingdon and G. J. Ferland, Astrophys. J. Lett. **516**, L107 (1999).

[4] J. B. Kingdon and G. J. Ferland, Astrophys. J. Suppl. Ser. **106**, 205 (1996).

[5] T. E. Cravens, Geophys. Res. Lett. **24**, 105 (1997).

[6] J. G. Wang, B. He, Y. Ning, C. L. Liu, J. Yan, P. C. Stancil, and D. R. Schultz, Phys. Rev. A **74**, 052709 (2006).

[7] H. J. Kim, R. A. Phaneuf, F. W. Meyer, and P. H. Stelson, Phys. Rev. A **17**, 854 (1978).

[8] C. C. Havener, E. Galutschek, R. Rejoub, and D. G. Seely, Nucl. Instrum. Methods Phys. Res. B **261**, 129 (2007).

[9] C. C. Havener, M. S. Huq, H. F. Krause, P. A. Schulz, and R. A. Phaneuf, Phys. Rev. A **39**, 1725 (1989).

[10] C. C. Havener, in *The Physics of Multiply and Highly Charged Ions, Vol. 2: Interactions with Matter*, edited by F. J. Currell (Kluwer Academic, Dordrecht, 2003), p.193–217.

[11] C. C. Havener, S. L. Hough, R. Rejoub, D. W. Savin, and M. Schnell, in *Proceedings of XXIV ICPEAC*, edited by Pablo D. Fainstein *et al.* (World Scientific, Singapore, 2006), pp. 522–530.

[12] C. C. Havener, M. A. Haque, A. C. H. Smith, and P. A. Zeijlmans van Emmichoven, in *VIth International Conference on the Physics of Highly Charged Ions*, edited by P. Richard, M. Stockli, C. L. Cocke, and C. D. Lin, AIP Conf. Proc. No. 274 (AIP, New York, 1993), p. 274.

[13] L. Folkerts, M. A. Haque, C. C. Havener, N. Shimakura, and M. Kimura, Phys. Rev. A **51**, 3685 (1995).

[14] D. G. Seely, H. Bruhns, D. W. Savin, T. J. Kvale, E. Galutschek, H. Aliabadi, and C. C. Havener, Nucl. Instrum. Methods Phys. Res. B **585**, 69 (2008).

[15] D. R. Schultz (private communication).

[16] R. A. Phaneuf, Phys. Rev. A **28**, 1310 (1983).

[17] P. C. Stancil (private communication).

[18] M. Kimura and N. F. Lane, Adv. At., Mol. Opt. Phys. **26**, 79 (1989).

[19] C. C. Havener, A. Müller, P. A. Zeijlmans van Emmichoven, and R. A. Phaneuf, Phys. Rev. A **51**, 2982 (1995).

[20] C. C. Havener, M. P. Nesnidal, M. R. Porter, and R. A. Phaneuf, Nucl. Instrum. Methods Phys. Res. B **56-57**, 95 (1991).

[21] R. Rejoub, M. E. Bannister, C. C. Havener, D. W. Savin, C. J. Verzani, J. G. Wang, and P. C. Stancil, Phys. Rev. A **69**, 052704 (2004).