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Publication Date

1986-10-01

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October 1986

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Presented at the Fourth International Symposium on The Production and Neutralization of Negative Ions and Beams, at Brookhaven National Laboratory, October 27-31, 1986

*Supported by U.S. DOE Contract DE-AC03-76SF00098 and USASDC MIPR W31RPD-63-A087.

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ABSTRACT

A high-charge-state plasma neutralizer for a beam of energetic H^- ions offers the potential of high optimum neutralization efficiency (~85%) relative to a gas target (50-60%), and considerably reduced target thickness. We have calculated cross sections for charge-changing interactions of fast H^- and H^0 in collision with highly charged ions using a semiclassical model for H^- , and the Classical-Trajectory Monte Carlo method plus Born calculations, to obtain correct asymptotic cross sections in the high-energy limit. Charge-state fractions as a function of plasma line density, and $f_0^{\max}$, the maximum H^0 fraction, are calculated using these cross sections; we find that $f_0^{\max} \approx 85\%$ for ion charge states in the range $1+$ to $10+$, and that target ion line density for $f_0^{\max}$ decreases approximately as the square of the plasma ion charge state. The maximum neutral fraction is also high for a partially ionized plasma. We have built a small multi-cusp plasma generator to use as a plasma neutralizer; preliminary results show that the plasma contains argon ions with an average charge state between $2+$ and $3+$ for a steady-state discharge.

INTRODUCTION

The use of an accelerated beam of H^- to provide an intense source of neutral H^0 requires the efficient removal of one electron from the H^- ion. A gas cell or a foil will produce a maximum H^0 yield of 50-60% at high energies. Laser photodetachment could, in principle, provide a very high H^0 yield, if a laser of sufficient power existed.

A dense plasma can be used as a neutralizer for an energetic H^- beam; cross-section data indicate that the conversion efficiency will be about 85%. A hydrogen plasma neutralizer has

* Supported by U.S DOE Contract DE-AC03-76SF00098 and USASOC MIPR W31RPD-63-A087.

been discussed by Grossman and by Berkner et al.,¹ and neutralizers for fast negative ions have been discussed by Schlachter.² A plasma neutralizer for fast negative ions³ has been studied experimentally by Dimov and co-workers and by Hershkovitch et al., and a recent publication in the Soviet literature by D'yachkov et al.⁴ has discussed apparent focusing of H^0 observed in the neutralization of 180-keV H^- in a Cs^+ plasma.

The purpose of our theoretical work is to calculate cross sections for single-electron-detachment

and double-electron detachment

for collisions of H^- with multiply charged ions. Ion charge states from $q = 1+$ to $10+$ and H^- energies from 250 keV/amu to 10 MeV/amu are considered. These cross sections are then used to predict H^0 yield and target thickness requirements for neutralizing H^- in partially and fully ionized plasmas.

THEORETICAL METHOD

The theoretical method used at the lower energies ($E \leq 1$ MeV/amu) was the four-body Classical-Trajectory Monte Carlo (CTMC) method. A program code was developed for this application which included the Coulomb interactions between the proton, its two electrons, and a fully-stripped multiply charged ion. The work led to the understanding of the collision mechanisms so that extension could be made to higher energies using a modified Born-approximation method.

The principal difficulty in implementing the CTMC method is the development of a suitable classical model for the H^- ion. It is well known that a classical two-electron atom is unstable and autoionizes unless constraints are placed upon the initial orbits for its electrons. It is crucial, however, that two electrons be explicitly included in the calculations in order to determine an accurate ratio of the single to double electron removal reactions. Statistical models based on one-electron Hartree-Fock calculations overestimate the importance of the double-electron-removal reaction. Such comparisons have been clearly demonstrated for collisions of multiply charged ions with helium.⁵ The direct application of the independent-electron model or the Born approximation predicts the σ_{-0} cross section for (1) should scale as $\sim q^2/E$, while the double-electron-removal cross section (2) should scale as $\sim q^4/E^2$. The E^{-2} dependence for double-electron removal is not confirmed in experiments⁶ using electrons as projectiles. Furthermore, the q^4 dependence leads to serious questions regarding the wisdom of using multiply charged ions in a plasma neutralizer since a large σ_{-+} cross section significantly degrades its efficiency.

Our application of the CTMC method is based on semiclassical quantization rules given by Einstein, Brillouin, and Keller.⁷ If one employs a self-consistent-field model for the H^- atom where each electron experiences an averaged potential due to the nucleus and the other electron, one can directly show that half-integer quantum numbers require the planes of the electron orbits to be offset 120° from one another and that the eccentricity of the orbits are equal to 0.866.

Within the context of a self-consistent-field model, the orbits of each electron are hydrogenic. Recalling the quantum-mechanical two-term spatial wavefunction for the H^- atom:

$$\Psi = N [e^{-\alpha r_1} e^{-\beta r_2} + e^{-\alpha r_2} e^{-\beta r_1}] , \quad (3)$$

it is possible to relate classically the parameters α and β to the effective charge experienced by each electron. Using Slater's rules, $\alpha = \beta = 0.6875$, and the total electronic energy calculated for H^- is -0.4727 a.u. (i.e. not bound!). The experimental value is -0.5277 a.u. Moreover, such values for α and β classically require each electron to be bound by 0.2363 a.u. ($\alpha^2/2$ and $\beta^2/2$), which is unacceptable since the first and second ionization potentials are 0.0277 a.u. and 0.500 a.u., respectively. Since classical electrons are distinguishable, it is possible to use effective charges of $\alpha = 0.2354$ and $\beta = 1.0000$ for the two electrons. With these values the experimental ionization potentials are reproduced, and quantum mechanical calculations using the split-shell wavefunction given by Eq. (3) yield an electronic energy of -0.5125 a.u., 72% closer to the experimental value than the single-parameter result.

A further consideration is that the classical calculations allow us to consider directly the effects of "shake-off" or "shake-up" in the collision. "Shake-off" is the phenomenon whereby the sudden removal of one of the electrons leaves the other electron in a configuration that is not an eigenfunction of the remaining ion or atom, resulting in further ionization. In "shake-up", this electron also has a finite probability of being found in an excited state.⁸ The excited-state production must be considered in the application to a plasma neutralizer. The excited atoms or ions will have a greatly enhanced possibility of ionization in subsequent collisions since their geometrical cross sections increase as n^4 , where n is the principle quantum number. Our calculations include the effects of both the direct impact ionization and "shake-up" and shake-off." For the application to modeling a plasma neutralizer we have assumed that any single-ionization events that leave the neutral H^0 in an excited level will be further ionized and should be classified as double ionization of the H^- projectile.

A model for the probability of double ionization is the product of the probability of removing the outer, loosely bound electron P_0 times the probability of removing the more tightly

bound inner electron P_I :

$$P_{2-ion} = P_0 P_I \quad . \quad (4)$$

The cross section is

$$\sigma_{-+} = 2\pi \int P_0 P_I \, bdb \quad . \quad (5)$$

However, since the limits of integration of Eq. (5) are restricted to small impact parameters by P_I where P_0 is approximately constant, we can rewrite Eq. (5) as

$$\sigma_{-+} = 2\pi P_0 \int P_I \, bdb \quad . \quad (6)$$

One can immediately see that Eq. (6) is simply

$$\sigma_{-+} = P_0 \sigma_{0+} \quad . \quad (7)$$

where σ_{0+} is the well-known single electron-removal cross section from neutral H^0 :

$$H^0 + \chi q^+ \rightarrow H^+ \quad . \quad . \quad . \quad (8)$$

Equation (7) must be further expanded upon to include the "shake-up" and shake-off" processes:

$$\sigma_{-+} = P_0 \sigma_{0+} + (1 - P_0) S \sigma_{0+} \quad . \quad (9)$$

The second term in Eq. (9) includes the possibility of ionizing the inner electron and not ionizing the outer electron, hence, the outer electron has a probability S of not finding itself in the ground state of the H^0 atom. The factor S equals 0.675. Note, a similar term exists for the "shake-up" of the inner electron but it is negligible. Equation (9) can be rewritten as:

$$\sigma_{-+} = (0.675 + 0.325 P_0) \sigma_{0+} \quad . \quad (10)$$

CTMC values for P_0 are given in Table I for charge states $q = 1, 2, 5$, and 10 and energies of 250 keV/amu, 1 MeV/amu, and 10 MeV/amu. The overall factor in Eq. (10) that relates the σ_{-+} and σ_{0+} cross sections is given in Table II. It is quite evident that "shake-up" is a very important process at the higher energies and cannot be ignored.

The CTMC calculations were performed at 250 keV/amu and 1 MeV/amu. Above 1 MeV/amu, the CTMC method loses validity due to the neglect of quantum tunneling. Correspondingly, above 1 MeV/amu, the Born approximation provides accurate cross sections. At 1 MeV/amu, the CTMC and Born-approximation cross sections for σ_{-0} are found to agree to within 20%, and the σ_{0+} values to within 30%. The Born cross sections of Kim and Inokuti⁹ were used in our studies. Tabulated values for the calculated cross sections are given in Table III.

Fig. 1 Calculated H^0 yield as a function of target ion (atom) line density for 1-MeV H^- in an Ar gas neutralizer and in a plasma neutralizer with ion charge state 1+ to 10+.

target thickness to obtain $f_0^{\max}$, as a function of plasma charge-state q for 1-MeV H^- ; figure 3 shows the energy dependence of π^{opt} and $f_0^{\max}$ for H^- in Ar and in plasmas with charge states 2 and 10.

For the case of an energetic H^- beam, where electron capture collisions can be neglected, it is easy to calculate $f_0^{\max}$ and π^{opt} :

$$f_0^{\max} = \left(\frac{\sigma_{-0}}{\sigma_{-0} + \sigma_{-+}} \right) \left(\frac{\sigma_{0+}}{\sigma_{-0} + \sigma_{-+}} \right)^{\gamma} \quad (11)$$

$$\text{where } \gamma = \frac{\sigma_{0+}}{\sigma_{-0} + \sigma_{-+} - \sigma_{0+}}$$

$$\pi^{\text{opt}} = \frac{1}{\sigma_{-0} + \sigma_{-+} - \sigma_{0+}} \ln \left(\frac{\sigma_{-0} + \sigma_{-+}}{\sigma_{0+}} \right). \quad (12)$$

The maximum neutral fraction $f_0^{\max}$ ranges from 84% to 86% for the cases studied. The line density required for maximum neutralization fraction decreases with increasing charge state of the plasma and increases with increasing beam energy.

The effect of partial ionization of the gas in a plasma neutralizer is shown in Fig. 4 for 1-MeV H^- in a mixture of Ar gas and a plasma with charge-state 5+; $f_0^{\max}$ and π^{opt} are shown as a function of the degree of ionization of the plasma (0 meaning pure Ar gas, 100% meaning pure $q=5+$). A high value of $f_0^{\max}$ is obtained even for a relatively low degree of ionization.

RESULTS

Charge-state fractions as a function of plasma line density for H^- incident on a plasma with ions in charge-state q and q electrons have been calculated by integrating a set of three first-order linear differential equations with effective cross sections obtained by adding q times the cross section for an electron collision to the cross section for collision with an ion. Examples are shown in Fig. 1 for 1-MeV H^- in Ar gas and in plasmas with charge states 1, 2, 5 and 10+. Figure 2 shows maximum neutral fraction $f_0^{\max}$ and π^{opt} , the

PLASMA-NEUTRALIZER DEVELOPMENT

The permanent-magnet-generated multicusp plasma device is capable of producing large volumes of uniform and high density plasma. Since the dipole fields confine the energetic electrons very effectively, discharge efficiency and ion charge-

Fig. 2 Charge-state dependence of maximum H⁰ fraction f_0^{max} and of target thickness to achieve f_0^{max} , π^{opt} , for 1-MeV H⁻ in an Ar-gas neutralizer ($q=0$) and in a plasma neutralizer with charge state q .

state distributions in the plasma can be optimized by using a "mixture" of primary electron energies. In addition, electro-static confinement of ions can be achieved by operation with a negative plasma potential or by using positively biased electrodes located between the line-cusps.

We have constructed and operated a small multicusp plasma generator containing high-charge-state ions for use as a plasma-neutralizer target. The plasma chamber

Fig. 3 Energy dependence of f_0^{max} and π^{opt} for H⁻ in an Ar-gas neutralizer and in a plasma neutralizer.

(15-cm-diam by 20-cm long) is made of copper and is surrounded externally by eight columns of samarium-cobalt magnets which form a longitudinal line-cusp configuration for primary-electron and plasma confinement. These magnet columns are connected at one of the end flanges by eight rows of magnets which converge to the axis of the chamber. In this configuration, a small field-free area is generated at the center of the flange. In order to determine charge-state distribution in the plasma, positive ions are

Fig. 4 Dependence of f_0^{max} and π^{opt} on degree of ionization of a plasma. O refers to pure Ar gas.

extracted from the plasma through a small aperture (1.5 mm-diam) located in this field-free region. The extracted beam is then analyzed by a compact magnetic-deflection mass spectrometer located just outside the plasma chamber.

Table IV summarizes the plasma parameters for operation with an argon plasma. The spectrometer output signal shows that the plasma is capable of producing argon ions with charge states as

Fig. 5 Photograph of plasma-neutralizer module.

high as $7+$, with an average charge state between $2+$ and $3+$ for a steady-state discharge of 250 V, 25 A. In order to reduce the operating discharge voltage, we are now investigating the use of other gases, for example, xenon. Initial results demonstrate that electron densities as high as $4 \times 10^{12} \text{ cm}^{-3}$ can be achieved with arc power of 150 V, 20 A in a low-pressure xenon discharge.

To achieve the proper line density for the neutralization of energetic H^- beams, a larger and longer modular-type multicusp plasma generator has been designed and fabricated. This neutralizer (25-cm-diam by 25-cm long) is bigger and therefore has a larger-field-free volume than the prototype neutralizer. Figures 5 and 6 show the appearance and the schematic of this new plasma-neutralizer module. The large number of ports around the chamber can provide easy access for the tungsten filaments or LaB_6 cathodes which are needed to generate a steady-state high-density

plasma. With this new plasma neutralizer, we plan to measure the magnetic-field distribution, the neutralization efficiency, the dependence of H^0 yield on plasma line density, and the angular divergence, for energetic H^- incident on this multiply charged plasma.

CONCLUSION

A theoretical method was developed to calculate the single- and double-electron-removal cross sections needed to model a plasma neutralizer. The maximum neutral H^0 fraction in a plasma neutralizer is $\sim 85\%$ and independent of energy for high-energy H^- . We are presently beginning to test a plasma target as a neutralizer for energetic H^- .

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Fig. 6 Schematic diagram of plasma-neutralizer module, configured for extraction of ions for charge-state-distribution measurement.

Table I. Probability P_0 of removing the outer electron on H^- by direct impact ionization in a collision with a fully-stripped multiply charged ion.

q	250 keV/amu	1 MeV/amu	10 MeV/amu
1	0.260	0.105	0.017
2	0.565	0.266	0.052
5	0.906	0.614	0.191
10	0.981	0.744	0.388

Table II. Calculated ratio of σ_{-+}/σ_{0+} which includes the possibility of "shake-up" and "shake-off."

q	250 keV/amu	1 MeV/amu	10 MeV/amu
1	0.760	0.709	0.681
2	0.859	0.761	0.692
5	0.969	0.875	0.737
10	0.994	0.917	0.801

Table III. Calculated cross section in cm^2 for reactions 1, 2, and 8, for H^- colliding with an ion in charge-state q.

q	σ_{-0}	σ_{0+}	σ_{-+}
250 keV/amu			
1	1.9(-15)	5.5(-17)	4.2(-17)
2	6.8(-15)	2.1(-16)	1.8(-16)
5	4.0(-14)	1.1(-15)	1.1(-15)
10	1.4(-13)	3.1(-15)	3.1(-15)
1 MeV/amu			
q			
1	4.6(-16)	1.8(-17)	1.3(-17)
2	1.9(-15)	7.4(-17)	5.6(-17)
5	1.2(-14)	4.6(-16)	4.0(-16)
10	4.6(-14)	1.8(-15)	1.7(-15)
10 MeV/amu			
q			
1	6.2(-17)	2.6(-18)	1.8(-18)
2	2.5(-16)	1.0(-17)	6.9(-18)
5	1.6(-15)	6.5(-17)	4.8(-17)
10	6.2(-15)	2.6(-16)	2.1(-16)

Table IV. Plasma parameters for plasma-neutralizer operation with Ar.

Discharge power:	250 V, 25 A
Electron density n_e :	$6 \times 10^{11} \text{ cm}^{-3}$
Gas pressure:	$5.3 \times 10^{-5} \text{ torr}$
Neutral density n_0 :	$1.75 \times 10^{12} \text{ cm}^{-3}$
n_e/n_0 :	0.34
Electron temperature T_e :	3.5 eV
Average charge state:	between 2 and 3

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This report was done with support from the Department of Energy. Any conclusions or opinions expressed in this report represent solely those of the author(s) and not necessarily those of The Regents of the University of California, the Lawrence Berkeley Laboratory or the Department of Energy.

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