Ionization rate coefficients of multiply ionized atoms*

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Ionization rate coefficients of He-like boron and carbon have been deduced from the time histories of the spectral lines emitted by B IV and C V ions in a small θ-pinch plasma. The radial electron density ($\sim 5\times 10^{15}$ cm^{-3}) and temperature (~ 220 eV) profiles were determined by 90° Thomson scattering. After making appropriate corrections for two-step ionization via the metastable $(1s2s)^3S_1$ level, theoretical estimates were found to agree with experimental results. A comparison of the above and previously measured ionization rates for various ions with existing theoretical predictions shows that the semiclassical theory of Burgess yields values that are in good agreement with experiment, especially at higher temperatures. For removal of $1s$ electrons, semiempirical rate coefficients are also in agreement with experiment, but are too large by a factor ~ 2 for other electrons.

I. INTRODUCTION

Knowledge of the lifetimes of various ionic stages of impurity atoms in high-temperature hydrogen or deuterium plasmas is very important in controlled nuclear fusion research for the estimation of radiation losses as well as in understanding, e.g., the physics of the solar corona (flares, etc.). The basic processes governing the ionic lifetime are collisional ionization and the various recombination processes—radiative, dielectronic, and three-body, whose relative importance is determined by the plasma conditions. It has been established in previous work that effective rate coefficients of ionization by electron collisions can be deduced from observed time histories of spectral lines emitted by ions in transient laboratory plasmas.[1-4]

In this paper, the underlying theoretical considerations for the determination of ionization rate coefficients are first briefly reviewed (Sec. II). In Sec. III the experimental methods are discussed and ionization rates for B IV and C V are presented. Of these, the rate for C V was measured earlier.[2] However, improved understanding of the population and depopulation mechanisms for the metastable level $(1s2s)\,^3S_1$ and its contribution to the total ionization rate necessitated a remeasurement and new interpretation, as discussed in Sec. II. Various semiempirical formulas have been proposed for the ionization rates, all of them giving essentially the same values. However, the semiclassical approximation[5] of Burgess was found to be much closer to the experimental values for most ions studied. Only for He- and H-like ions are the semiclassical theory and semiempirical formulas in agreement. A general comparison is given in Sec. IV.

II. THEORETICAL CONSIDERATIONS

A detailed description of the method for the determination of ionization rate coefficients was given in Ref. 3. Basically, the method involves solving the coupled rate equations for the various ion densities [Eqs. (3) in Ref. 3], using measured electron densities and electron temperatures as well as approximate theoretical ionization rate coefficients having the correct temperature dependence. Then, using the relation for corona excitation equilibrium [Eq. (4) of Ref. 3], the time histories of the emission lines are predicted. This is accomplished for the present investigations using a computer program.[3,6] The determination of improved ionization rate coefficients finally involves changing the ionization coefficients in the coupled rate equations until the predicted time histories match with the experimentally observed time histories. What is thus actually measured is therefore an effective ionization rate, i.e., a sum of the ionization rates from the ground state, including inner-shell ionization, and all of the populated excited states. This also assumes that all recombination processes are negligible, which is indeed the case for our experimental conditions, i.e., electron temperatures substantially higher than those corresponding to corona ionization equilibrium.

For heliumlike ions the metastable triplet levels with principal quantum number $n=2$ may contribute to the total ionization rate, depending on the electron density. This effect has been discussed in the modified corona model for He-like ions in Ref. 2 and was reviewed in detail in Ref. 7. Using the notation of Ref. 2, the effective ionization coefficient may be written

$$I_{eff} = (I_1 + \alpha X_{31}). \qquad (1)$$

Here I_1 describes the ionization from the ground state, X_{31} is the excitation rate coefficient to $n=2$ triplet states from the ground state, and α is the branching ratio for ionization from $n=2$ triplet levels. It is estimated by

$$\alpha = I_3 N/[A_{13} + (I_3 + X_{3\geq} N)], \tag{2}$$

where I_3 is the $n=2$ triplet-level ionization coefficient, A_{13} is the intercombination-line transition probability, and $X_{3\geq}$ is the collisional transfer rate coefficient from $n=2$ triplet levels to singlet levels of $n=3$ and higher. In contrast to Ref. 2, transfer from triplets to singlets in $n=2$ levels is neglected. This is discussed in detail in Ref. 7, and α was estimated by using the expressions (4-6-3) and (4-6-14) in Ref. 7. Following Ref. 2, the total excitation rate coefficient for $n=2$ triplet levels X_{31} was taken to be as $X_{21}/1.8$, where X_{21} is the total excitation coefficient to the $2\,^1S$ and $2\,^1P$ levels. The coefficient X_{21} had been found[2,8] to be consistent with the effective Gaunt factor approximation,[9] which we will therefore use.

The ionization from the ground state represented by I_1 is estimated both by a semiempirical formula[3] and by the semiclassical approximation introduced by Burgess,[5] which is called the exchange collisional and impact parameter method[10] (ECIP). We note, finally, that we need not distinguish between $2\,^1S$ and $2\,^1P$ levels, because collisional transfer from $2\,^1S$ to $2\,^1P$ is so rapid[7] that $2\,^1S$ excitation is equivalent to direct excitation to $2\,^1P$. For the $n=2$ triplet levels, we can safely assume[7,11] statistical populations for the ions and plasma conditions in the present measurement.

III. MEASUREMENT OF RATE COEFFICIENTS

The plasma was generated in a 15-kJ θ-pinch machine, detailed descriptions of which can be found elsewhere.[3,12] The main bank was discharged when an antiparallel (with respect to the main field) 600-G bias field was present. A 0.6-kJ preheater was fired 16 μsec earlier than the main bank.

The discharge tube was filled with 11 mTorr H_2 base gas and a small percentage of the impurity. Boron was introduced into the chamber by using a mixture of Diborane (B_2H_6) with hydrogen, resulting in 0.5 at.% of boron in 11 mTorr H_2. Similarly, methane was used to introduce carbon. A plasma mixture with 2 at.% carbon added to 11 mTorr H_2 was investigated. The plasma was studied in the first half cycle of the discharge, i.e., for 4.5 μsec after the main discharge.

Electron densities and temperatures were measured for each plasma condition using 90° Thomson scattering. The setup was as described in Ref. 2. Both temporal and radial profiles were obtained. The plasma forms into a cylindrical column with about 2 cm radius. The plasma has large radial density and temperature fluctuations at early times, i.e., before 1.0 μsec, as it bounces radially in response to the magnetic piston. These fluctuations tend to smooth out at later times. Densities and temperatures were averaged over the column cross section in the midplane, and Fig. 1 shows the results for the 2-at.%-carbon mixture.

For the early times, before 1.5 μsec, two different averages are shown. The dotted line is a linear temperature average, with no weight factors put in. This is used in our present work, as it was found in previous experiments[13] that at these early times impurity ions are not thermalized. They would bounce[14] in the magnetic well, and are not magnetized. The ions were found[13] to acquire up to twice the piston speed. The continuous line is the average temperature across the cylindrical column cross section in the midplane, with the electron density weight factor put in. The ions, if fully magnetized (as the electrons are) would see this temperature. The results from using these two averages are discussed in Sec. IV. The density average is the average density over the column cross section in the midplane.

The plasma reaches the peak temperature by 1.5 μsec and cools rapidly after 2.75 μsec as it goes to the walls. The period between 1.5 and 2.5 μsec is ideally suited for ionization rate mea-

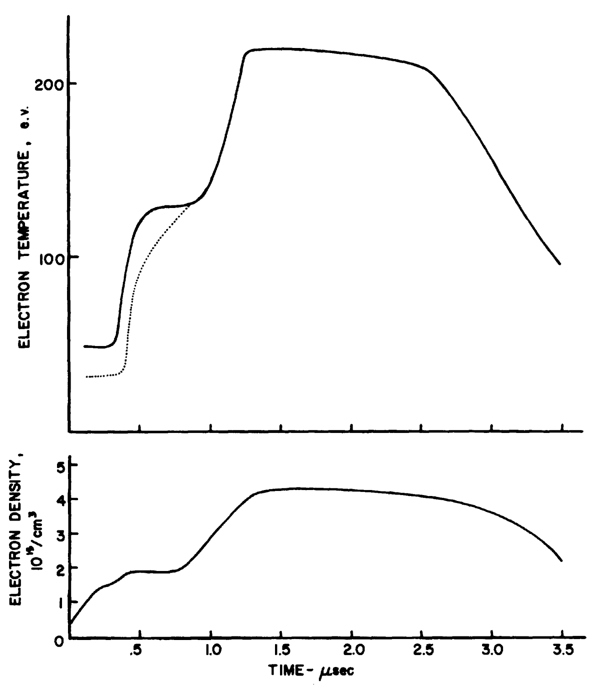

FIG. 1. Measured electron density and temperature profiles; 2-at.%-carbon, 11-mTorr-H_2 case. Estimated mean error ~5%.

surements. The addition of impurities reduced the temperature by 15–20% and the density by 10–15%. The lifetime of the hot plasma was also effected. For example, in the case of boron the plasma cooled to 50% of its peak temperature by 2.6 μsec, possibly owing to a faster decay of the reverse field configuration near the end of the plasma column. It was therefore important to obtain the plasma parameters for each individual case.

Spectroscopic observations were made end on with a 2-m grazing incidence spectrometer and a $\frac{1}{4}$-m monochromator. The 2271-Å line of C V was always observed side on in each shot. Its time history served as a monitor for the reproducibility of the plasma conditions and also in the analysis of C V ionization rates.

Side-on observations are generally preferable, because one then avoids the cooler or low-density end regions of the plasma column. For this reason end-on time histories often have slower decay rates. However, time histories of higher ionization stages tend to be the same end on or side on, as these ions occur only in the hot central portion of the plasma column. This is evidenced in the present experiment by the observation of identical decay rates for the C V 2271-Å line in the two directions.

The time histories of all detectable emission lines connecting to the ground states of C IV, C V, C VI, B IV, and B V were measured.[15] An average time history was thus obtained for these ionization stages. The standard error of the mean over any portion of the time history was less than 5% of the peak intensity. The times of the peak intensities, and the half-peak-intensity times on either side of the peaks, were reproducible within 5% or better. The optical depth correction for the resonance lines was found to be negligible.

Figure 2 shows the experimental time histories and the computed time histories made to match them by choosing appropriate ionization rates. The computation was performed including the recombination processes—dielectronic[16] and radiative[17,18]—which could be important at our densities and temperatures. However, even the dielectronic recombination, which was contributing most, was always at least an order of magnitude slower than ionization rates for the ions under consideration. For early times, corresponding to C IV and B III, and late times, corresponding to the decay of B V and C VI, the time histories were more influenced by the variations in plasma column length, electron density, and temperature, and did not match well with computed time histories. For the early ions lower effective ionization rates had to be used to match the computed starting times of occurrences and the earlier part of the rise of He-like ions with the observations in the experiment. Thus the conditions in the computations were made to simulate the experiment during these times. It was found from the computed populations that the ionization rates of He-like ions alone govern the remainder of their time histories. Evaluation of the various terms in Eq. (7) of Ref. 3 showed that the time histories of C V and B IV are not influenced by the first three terms, which describe intensity variations from changes in plasma length, density, and temperature, a necessary condition for a good determination of ionization rates.

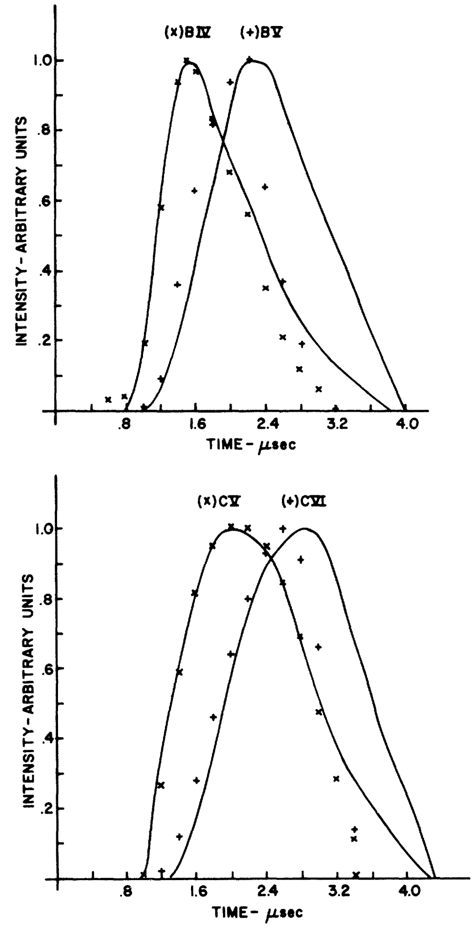

FIG. 2. Matched-time histories. Continuous lines are experimental time histories. Mean error over any portion was less than 5% of peak intensity. Marks are points from computed time histories.

IV. RESULTS AND DISCUSSION

Our experimental (best-fit) ionization rate coefficients are given in the last column of Table I. The effective calculated rate coefficients and the relevant rate coefficients used in the calculation

TABLE I. Collisional rate coefficients (in units of 10^{-10} $cm^3 sec^{-1}$) and branching ratio α for triplet ionization.

Ion	I_1	X_{31}	I_3	$X_{3\geq}$	α	I_{eff} Theor.	I_{eff} Expt.
B IV	2.09	1.33	33.5	12.5	0.68	3.0	2.4 ± 0.7
C V	0.60	0.62	15.5	6.9	0.39	0.8	0.8 ± 0.2

are given in the preceding columns. For the ground-state ionization coefficient I_1 the semiempirical values[3] were used. [Note that for He- and H-like ions the ECIP rate coefficients[10] are in agreement with these values (within 10%).] The intercombination transition probability is taken from Ref. 19 and is related[2] to the total $n=2$ triplet population by dividing by 4. The branching ratios α in Table I correspond to typical times (1.7 and 2.3 μsec, respectively) during the decay of each ion. For the corresponding plasma conditions ($kT \sim 200$ eV, $N \sim 4.9\times10^{15}$ cm^{-3} and $kT \sim 215$ eV, $N = 4.2\times10^{15}$ cm^{-3}) ~68% of the excitations to $n=2$ triplets lead to ionization in the case of B IV, whereas in the case of C V this ratio is 39%. Nevertheless, the total contribution due to two-step ionization via $n=2$ triplet levels is the same in both cases, namely, about 30%. The experimental results for C V are in agreement with results in Ref. 2. (No previous measurements have been made for B IV.)

The ratio of resonance line and intercombination line intensities was measured in the case of C V. These results also agreed with Fig. 5 of Ref. 2.

Based on the sensitivity of matching the time histories to the ionization rates and the mean fluctuation of the time histories from shot to shot, an error of 25% in the case of C V was estimated for the experimental ionization rate given in the last column of Table I. However, it was found that the ionization rate for B IV was sensitive to the early-time behavior of electron temperature, whereas the ionization rate for C V was practically independent of it. If the full line is used for the early-time behavior of the temperature, the ionization rate for B IV would be ~30% lower than that given in the last column. From these considerations an error of ~30% was estimated for the experimental ionization rate of B IV. Possible errors of 5–10% in the density and temperature determination over the remaining portions of Fig. 1 do not significantly influence the results, because the matching was not sensitive to such changes.

V. GENERAL COMPARISON WITH THEORY

The semiclassical theory of Burgess[5] (ECIP) was found for various ions and at high temperatures to be in better agreement with experimental results.[3,4,20] than the predictions based on semiempirical formulas (see Table II). Semiempirical values were calculated using the formula in Ref. 3, which is a fit to Lotz's[21] semiempirical predictions, and the formula of Hinnov,[22] which yields very similar results. Both semiempirical estimates are in essential agreement with semiclassical results for H- and He-like ions, whereas they are mostly a factor of ~2 higher for other ions.

In Table II the experimental ionization rates for various ions, measured mainly at temperatures half the ionization threshold or higher, are compared with semiempirical[21] and semiclassical[5,10] predictions. The semiempirical predictions are a factor of ~2 higher, whereas the semiclassical values are in fair agreement with experiment.

TABLE II. Ionization rates (in units of 10^{-9} cm^3/sec).

Ion	kT/E_i [a]	I_{expt}	$I_{Burgess}$ (semiclassical theory)	I_{Lotz} (semiempirical)
Fe VIII	0.73	0.30 [b]	0.35	0.62
Fe IX	0.53	0.27 [b]	0.21	0.44
Fe X	0.54	0.18 [b]	0.15	0.34
Ar VIII	1.01	0.2 [c]	0.17	0.33
	1.81	0.52 [c]	0.3	0.87
Ne VII	0.96	0.29 [d]	0.22	0.42
O V	1.23	0.7 [d]	0.74	1.35
O VI	1.45	0.35 [d]	0.31	0.59
N V	2.04	0.63 [d]	0.67	1.26
C IV	2.33	1.52 [d]	1.29	2.53

[a] kT is the electron temperature, and E_i is the ground-state ionization potential.
[b] From Ref. 4.
[c] From Ref. 20.
[d] From Ref. 3.

This comparison could not be extended to the experimental results of Hinnov[1] for various neon ions, owing to the uncertainties in the temperature measurements.

VI. SUMMARY AND CONCLUSIONS

Ionization rate coefficients for He-like C V and B IV ions were obtained experimentally with an estimated error of 25–30%. Agreement with predicted values, based in part on the present understanding of the contribution of two-step processes to total ionization rates, is within the estimated error limits in the case of C V and B IV. It is also found from a general comparison for ions containing other than 1*s* electrons that semiclassical predictions based on Burgess's ECIP approximation[5] are in better agreement than semiempirical values[21,22] with experimental results.

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