Experimental and theoretical cross sections for electron-impact ionization of Ti^{5+}

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Absolute cross sections for electron-impact ionization of Ti^{5+} have been measured from below threshold to 1500-eV collision energies. Distorted-wave calculations including direct ionization and excitation autoionization from the $3s^23p^5$ ground state and from the $3s^23p^43d$ excited configurations have been performed. Comparison of experiment and theory indicates that about 33% of the incident ions were in metastable configurations. Ionization rate coefficients and fitting parameters derived from the experimental results are also presented.

I. INTRODUCTION

For a long time studies of the properties of highly charged ions have been encouraged by diverse plasma physics communities. Indeed, atomic data are necessary for astrophysics, ion source development, and magnetic and inertial confinement fusion. Moreover, the recent demonstration of x-ray lasing[1,2] has increased the need for understanding the processes of ionization and recombination.

An interesting aspect of electron-impact ionization is the contribution of indirect processes to the cross section. Previous experimental and theoretical studies[3] have demonstrated their importance. In particular, excitation autoionization can significantly enhance the total-ionization cross section. For instance, measured Ti^{3+} ionization cross sections were a factor of 10 higher than the direct ionization calculations.[4] Qualitative agreement was found when the effects of excitation autoionization were included in the calculations.[5] Theoretical methods[5-7] have been improved over the years and allow a fair quantitative agreement with the measured cross section. In the case of Ti^{2+}, however, the discrepancy with available theory[7] remains large.[8] Moreover, the presence of ions in metastable configurations in experiments strongly modifies the physics to be included by theory, especially in the case of metallic ions. In recent studies of the iron isonuclear sequence, calculations[9] for Fe^{9+} are in reasonable agreement with experiment[10] only when excitation autoionization from metastable states of the $3p^43d$ excited configuration are included.

Since neither the titanium isonuclear sequence nor the chlorine isoelectronic sequence (which includes Fe^{9+}) is well understood, the cross section for ionization of Ti^{5+} has been investigated both theoretically and experimentally. In Sec. II we discuss the experimental arrangement and in Sec. III we briefly describe the theoretical method used to calculate the ionization cross section. Experimental and theoretical results are presented and compared in Sec. IV. Because many users of such data are interested in ionization rates, Maxwellian rate coefficients based on the present cross-section measurements have been calculated and are presented in Sec. V. Finally, some conclusions are given in Sec. VI.

II. EXPERIMENTAL SETUP

In order to establish absolute cross sections for electron-impact ionization, a number of parameters have to be measured accurately. In the case where electron and ion beams cross at 90°, the cross section σ at the collision energy E is given by the expression[10]

$$\sigma(E)=\frac{Rqe^2v_iv_eF}{I_iI_e(v_i^2+v_e^2)^{1/2}D}\ , \qquad (1)$$

where R is the signal count rate, qe is the charge of the incident ions, e is the electron charge, v_i and v_e are ion and electron velocities, I_i and I_e are the ion and electron beam currents, D is the detecting efficiency of a signal event, and F is the form factor which takes account of the spatial overlap of the two beams.

A detailed description of the apparatus has been provided in a previous publication.[11] Here, we present a brief overview of the experimental arrangement. The experiment was performed at the Oak Ridge National Laboratory Electron Cyclotron Resonance (ORNL-ECR) source.[12] Ions of elements existing as permanent gases are straightforward to produce with such a source. However, in the case of titanium, as well as for many metallic elements, a solid feed technique is used in order to generate ions. Indeed, for the experiment, a 0.025-mm-thick titanium foil was introduced into the ECR plasma, where it was heated by electron impact, evaporating titanium ions. Nitrogen gas was also inserted in the source to regulate and maintain the gas pressure in the plasma in the absence of metal vapor. A 0.064-mm-thick sample has also been tried, but the thermal time constant was too high and the titanium vapor was not sufficiently dense to produce enough titanium ions. The vaporization rate was controlled by changing the foil position, tuning the

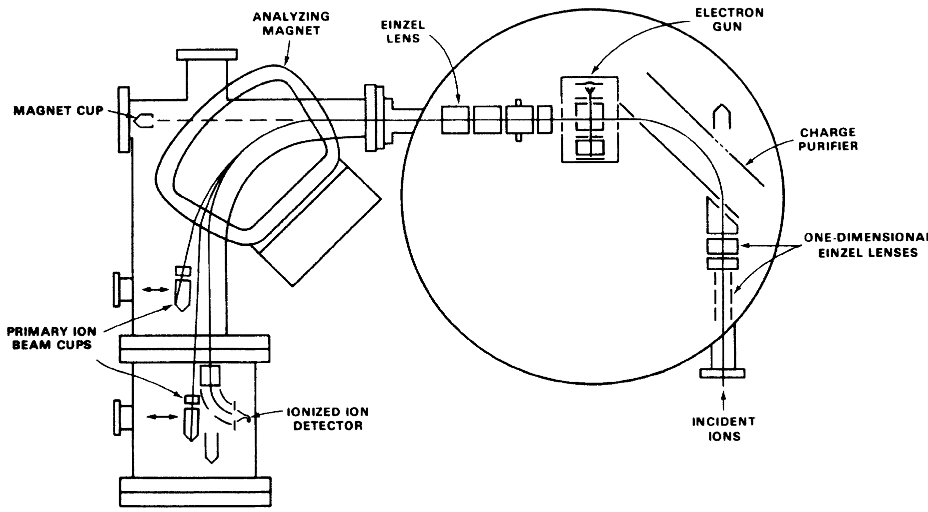

FIG. 1. Schematic of the interaction chamber. The drawing is to scale. The inside diameter of the main chamber is 24 in. For simplicity, the signal ions final 90° deflection out of the analyzer plane is represented as being in the analyzer plane.

source magnetic field, or adjusting the microwave power. The average Ti^{5+} ion current extracted from the source was about 10^{-6} A.

The apparatus used to perform the measurements is shown schematically in Fig. 1. The ions are extracted at 10-kV potential from the source. The desired ions are selected by a magnetic analyzer and transported to the interaction chamber. Electron and ion beams cross in the center of the electron gun, which is similar to that described by Taylor *et al.*[13] Further ionized ions are then separated from the parent beam by a magnetic analyzer. Finally, the signal ions are electrostatically deflected out of the analyzer plane and detected by a channel-electron-multiplier detector. The signal event rate is obtained by measuring the detector count rate and subtracting the background (count rate when the electron beam is absent). The global count rate efficiency is 0.95, including the pulse transmission of the electronics, the detection efficiency of the detector, and the transmission of the signal ions from the interaction region to the detector. The parent ion and electron beams are collected in two Faraday cups and both currents are integrated during each measurement. Finally, the form factor is derived from beam profile measurements that were achieved by moving a narrow slit across both beams and measuring the transmitted currents.

Experimental parameters obtained at 300 eV, near the peak of the cross section are reported in Table I. At that

TABLE I. Experimental parameters at 300-eV electron energy.

Electron current (mA)	2
Ion current (nA)	95
Background count rate (sec^{-1})	88
Signal count rate (sec^{-1})	500
Form factor (cm)	0.46

energy, the (electrical) ion current (95 nA) was particularly high. The ion beam intensity in the interaction region varied from day to day, from 20 and 70 nA. The electron beam intensity was of the order of 2 mA, and the energy spread was between 1 and 2 eV full width at half maximum (FWHM), depending on the beam energy. The pressure in the chamber was about 2×10^{-9} Torr.

III. THEORETICAL METHODS FOR Ti^{5+} IONIZATION

The electron-impact ionization cross section of Ti^{5+} has also been estimated theoretically. In the case of Ti^{5+}, the effects of interference between the direct and indirect processes, radiative decay of the core-excited autoionizing states, and energy-level splitting within the configurations are all assumed to be small. In these conditions, the total electron-impact single-ionization cross section may be given by

$$\sigma_{\rm tot}=\sum_{nl}\sigma_{\rm dir}(nl)+\sum_{nl,n'l'}\sigma_{\rm exc}(nl\to n'l') , \tag{2}$$

where $\sigma_{\rm dir}(nl)$ is the direct ionization cross section from the nl subshell of the initial configuration and $\sigma_{\rm exc}(nl\to n'l')$ is the excitation cross section from a subshell nl of the initial configuration to a particular subshell $n'l'$ of a core-excited configuration. The total cross section from the ground configuration of Ti^{5+} is given by

$$\sigma_{\rm tot}(3s^23p^5)=\sum_{l=0}^{1}\sigma_{\rm dir}(3l)+\sum_{l=1}^{2}\sigma_{\rm exc}(2p\to3l) , \tag{3}$$

while that from the first excited configuration of Ti^{5+} is given by

$$\sigma_{\rm tot}(3s^23p^43d)=\sum_{l=0}^{2}\sigma_{\rm dir}(3l)+\sum_{l=1}^{2}\sigma_{\rm exc}(2p\to3l)+\sum_{l=0}^{3}\sigma_{\rm exc}(3s\to4l) . \tag{4}$$

TABLE II. Excitation cross sections to autoionizing configurations in Ti^{5+}.

Excitation	Threshold energy (eV)	Threshold cross section (10^{-18} cm^2)
	$3s^2 3p^5$ ground configuration	
$2p \rightarrow 3p$	432.13	0.043
$2p \rightarrow 3d$	470.74	0.345
	$3s^2 3p^4 3d$ excitation configuration	
$3s \rightarrow 4s$	91.66	1.963
$3s \rightarrow 4p$	99.22	0.393
$3s \rightarrow 4d$	110.45	0.377
$3s \rightarrow 4f$	117.46	0.358
$2p \rightarrow 3p$	432.31	0.085
$2p \rightarrow 3d$	472.26	0.308

The direct and excitation-autoionization cross sections were obtained in a configuration-average distorted-wave approximation.[9] The $2s$ and $2p$ are not included in direct ionization since they contribute to double ionization. For the ground configuration, excitations from the $3s$ to $4l$ subshells are to bound orbitals and are not included in Eq. (3).

The excitation cross sections $2p \rightarrow 3l$ ($l=1,2$) for the ground configuration and $2p \rightarrow 3l$ ($l=1,2$) and $3s \rightarrow 4l$ ($l=0,1,2,3$) for the first excited configuration are given in Table II. The energy eigenvalue and bound radial orbital calculations needed to evaluate the cross sections were made using Cowan's Hartree-Fock atomic wave-function code.[4]

IV. RESULTS AND DISCUSSION

The experimental values of the electron-impact ionization cross section of Ti^{5+} are listed in Table III and plotted in Fig. 2 as a function of the collision energy. The relative uncertainties in the table are reported at the one-standard-deviation level and are of the order of 1% of the peak cross section. The error bars are smaller or equal to the point size and so they have not been reproduced on the graph. The uncertainty in the absolute magnitude of the curve near the peak cross section is 7% at good confidence level (equivalent to 90% confidence level on statistical uncertainties).

In Fig. 2, the experimental data are compared to theoretical calculations using the configuration-average distorted-wave approximation described in the previous section.[9] The two lower curves represent the direct ionization (dashed curve) and direct plus excitation-autoionization (solid curve) cross sections assuming that the ions are initially in the ground configuration. The two upper curves correspond to the same processes assuming that 100% of the ions are initially in the $3s^2 3p^4 3d$ excited configuration. The theoretical calculations include the direct ionization cross sections of the $3l$ subshells as well as excitation-autoionization contributions arising from $3s \rightarrow 4l$ transitions for the first excited configuration and from $2p \rightarrow 3l$ transitions for both ground and excited configurations.

Comparing experiment and theory, one can see that the ion beam contained a non-negligible percentage of ions in metastable configurations which contributed to the cross section. The onset of the cross section is found well below the predicted energy for removal of an outer $3p$ electron from the ground-state ion. The threshold occurs at approximately 85 eV, which corresponds to the energy needed to remove the $3d$ electron from the $3p^4 3d$ excited configuration (38.4 eV above the ground state).

For the first excited configuration, the contribution of excitation autoionization occurs almost from threshold.

TABLE III. Experimental cross sections for ionization of Ti^{5+}. Relative uncertainties are quoted at the statistical one-standard-deviation level or equivalent.

Energy (eV)	Cross section (10^{-18} cm^2)
75.9	-0.068 ± 0.071
80.7	0.10 ± 0.08
86.0	0.288 ± 0.063
95.6	0.80 ± 0.08
105.7	1.04 ± 0.07
115.3	1.38 ± 0.07
125.0	2.26 ± 0.07
135.1	3.61 ± 0.07
144.7	4.51 ± 0.07
154.9	5.05 ± 0.08
164.3	5.51 ± 0.06
174.4	5.79 ± 0.06
184.0	6.05 ± 0.06
194.3	6.39 ± 0.06
214.1	6.84 ± 0.09
233.9	7.20 ± 0.08
253.0	7.34 ± 0.08
272.9	7.51 ± 0.06
292.9	7.36 ± 0.03
317.5	7.28 ± 0.05
342.7	7.29 ± 0.04
367.3	7.20 ± 0.04
391.8	7.09 ± 0.04
405.0	7.41 ± 0.08
420.0	7.20 ± 0.08
441.2	7.24 ± 0.03
460.1	7.60 ± 0.09
479.5	7.37 ± 0.09
489.9	7.39 ± 0.02
499.5	7.58 ± 0.09
519.0	7.60 ± 0.08
539.0	7.28 ± 0.04
588.0	7.04 ± 0.05
637.2	6.96 ± 0.04
687.0	6.63 ± 0.02
736.3	6.48 ± 0.03
785.3	6.32 ± 0.03
834.0	6.19 ± 0.03
884.0	6.06 ± 0.03
984.0	5.99 ± 0.02
1082.0	5.58 ± 0.07
1179.0	5.29 ± 0.07
1273.0	4.94 ± 0.05
1372.0	4.89 ± 0.09
1467.0	4.57 ± 0.07

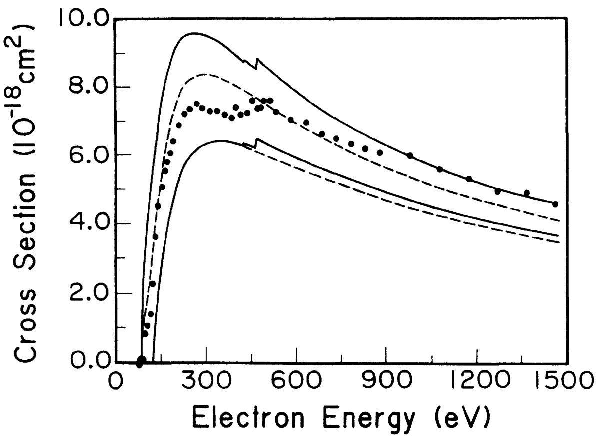

FIG. 2. Electron-impact ionization cross section for Ti^{5+}. Solid points are the present measurements; relative uncertainties at the one-standard-deviation level are smaller than the plotted points and have not been included in the graph. The two lower curves represent direct ionization only (dashed curve) and direct ionization plus excitation autoionization (solid curve) assuming the ions are initially in the ground state. The two upper curves correspond to the same processes for 100% of the ions initially in the $3s^23p^43d$ metastable configuration.

For both the ground and excited configurations, the $2p \rightarrow 3d$ dipole transition has the largest single contribution and provides a small enhancement around 470 eV. Excitation autoionization is predicted to have a small contribution because the outer shell is filled with five electrons. For the same reason, an indirect ionization mechanism such as REDA (resonant excitation double autoionization) is not expected to be seen in the cross section. Another structure around 550 eV may be due to the direct ionization of a $2p$ electron. However, one would expect that an excited ion formed in such a way would autoionize to Ti^{7+} so that no contribution would be seen in this experiment.

The percentage of ions initially in the excited configuration in the beam has been estimated in the following way. The theoretical cross section has been scaled fixing a fraction of the ions initially in metastable states of the excited configuration and the remainder in the ground state in order to bring the theory into good agreement with experiment. For Ti^{5+}, a 33% metastable state fraction was found to make theory and experiment agree very well up to the onset of excitation autoionization from the ground state. However, the theoretical tail slightly underestimates the data.

Electron-impact ionization cross sections for chlorine-like ions have also been calculated by Younger[15] using the distorted-wave Born exchange approximation. The results for Ti^{5+} are not presented here because they do not include the excitation-autoionization process and the cross section is calculated only for ions initially in the ground state. However, in the same conditions, the cross section obtained was about 9% lower than the calculations presented here.

V. RATE COEFFICIENTS

The cross-section measurements have been converted to rate coefficients using a computer program developed by the Controlled Fusion Atomic Data Center at Oak Ridge National Laboratory. This program also provides convenient fits of these rate coefficients. The method of calculation and fitting has been described previously.[10,16] Because of the finite energy range over which the cross section has been measured, the highest-energy experimental data were extrapolated up to 30 keV by the $\ln E/E$ energy-dependence scaling predicted in the Bethe-Born approximation. Sample ionization rate coefficients obtained for Ti^{5+} are listed in Table IV as a function of selected energies kT. Their natural logarithms have been fitted to a Chebyshev polynomial expansion following the method reported by Cox and Hayes.[17] The rate coefficients can be obtained at any value of kT from $E_{\min}=10$ eV to $E_{\max}=3000$ eV using the formula

$$\alpha(kT)=\exp\left[\tfrac{1}{2}a_0+\sum_{r=1}^{8} a_r T_r(x)\right], \tag{5}$$

where the rate coefficient α is in 10^{-10} cm^3/s, kT is in eV, $[\mathrm{Tr}(x)]$ is a direct expansion of Chebyshev polynomials[18] of the first kind and

$$x=\ln\left[\frac{(kT)^2}{E_{\min}E_{\max}}\right]\Big/\ln(E_{\max}/E_{\min}) . \tag{6}$$

The rate coefficients fitting parameters a_r ($r=0,1,\ldots,8$) obtained for Ti^{5+} are the following:

TABLE IV. Ionization rate coefficients for Ti^{5+} (in 10^{-10} cm^3/s) at selected values of kT (in eV), derived from the experimental data.

kT	Rate coefficient
10.0	0.0033
20.0	0.3426
30.0	1.9285
40.0	4.823
55.0	10.57
75.0	18.92
86.0	23.38
105.7	30.78
154.9	45.77
194.3	54.81
253.0	64.85
292.9	69.91
342.7	74.86
405.0	79.46
499.5	84.09
588.0	86.74
687.0	88.45
785.3	89.32
884.0	89.61
984.0	89.54
1082.0	89.19
2000.0	82.26
3000.0	74.81

$$a_0=-41.9880,\quad a_1=3.342\,05,\quad a_2=-2.769\,04\ ,$$
$$a_3=1.074\,48,\quad a_4=-0.394\,464,\quad a_5=0.120\,767\ , \tag{7}$$
$$a_6=-0.038\,97,\quad a_7=-0.003\,499,\quad a_8=0.004\,805\,5\ .$$

Note that the rate coefficient is the exponential of the standard Chebyshev polynomial expansion. A computationally fast method of evaluating Chebyshev polynomials has been devised by Clenshaw,[19] and a sample program based on Clenshaw's algorithm is available.[20]

VI. CONCLUSION

Experimental and theoretical cross sections for electron-impact ionization of Ti^{5+} have been presented. The comparison of calculations and measurements shows that a large component of the ion beam (approximately 33%) was initially in the metastable states of the $3s^23p^43d$ configuration. The presence of metastable ions increases the ionization cross section by about 20% near its peak. The excitation-autoionization contribution represents a small contribution to the total cross section if the ions are initially in the ground state. However, the contribution is significant for the first excited-state configuration. A distorted-wave ionization calculation, which includes the effects of excitation autoionization and assumes a 33% metastable component in the incident ion beam, is in good agreement with the experimental results.

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