INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS B: ATOMIC, MOLECULAR AND OPTICAL PHYSICS

J. Phys. B: At. Mol. Opt. Phys. **37** (2004) 4387–4395 PII: S0953-4075(04)84440-7

Electron-impact ionization of Ti^{3+} ions

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Received 23 July 2004, in final form 4 October 2004
Published 26 October 2004
Online at stacks.iop.org/JPhysB/37/4387
doi:10.1088/0953-4075/37/21/011

Abstract

Absolute cross sections for electron-impact single ionization of potassium-like titanium have been measured from threshold to 1000 eV using a crossed-beams experimental set-up. A 0.5 eV resolution energy-scan technique revealed structures in the cross section in the range from 40 eV to 150 eV due to dominant contributions of indirect ionization mechanisms. A large fraction of the cross section is due to excitation–autoionization proceeding via intermediate excited states $3p^5(3d^2\,{}^3F)\,{}^2F$, $3p^5(3d^2\,{}^3P)\,{}^2P$, $3p^5(3d^2\,{}^3F)\,{}^2D$ which subsequently decay by super-Coster–Kronig transitions. The results of the measurements are in satisfactory agreement with previous advanced theoretical calculations.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Electron-impact ionization is one of the most fundamental atomic collision phenomena and also one of the most important processes in plasmas. Cross sections for electron-impact ionization are needed for the detailed understanding and modelling of any technical or natural plasma and therefore have important applications in astrophysics and in fusion research [1, 2].

Because of its relevance in applications and its appeal as a quasi-one-electron system with one 3d electron outside a closed Ar-like configuration, potassium-like Ti^{3+} has been the target of substantial efforts to study its behaviour in fundamental interactions with electrons and photons. Much of the existing work on ionization of Ti^{3+} is theoretical because experiments using beams of Ti^{3+} ions have been handicapped by either low beam intensities or by the presence of ions in autoionizing metastable states. Such ions are responsible for excessively high backgrounds in ionization experiments employing the technique of colliding beams.

The first and so far only successful experimental study on electron-impact single ionization of Ti^{3+} was reported by Falk *et al* [3, 4]. This experiment stimulated a number of theoretical

studies which employed a variety of different approaches such as a Coulomb–Bethe method [5], full distorted-wave calculations [6] and *R*-matrix theory with different sizes of basis sets [7–9]. The results of these theoretical approaches substantially differ from one another and none of the calculations could reproduce the experimental data of Falk *et al* in a satisfactory manner. Later, a systematic experimental study of single, double and triple ionization of Ti^{q+} ions with q ranging from 1 to 7 was conducted by Hartenfeller *et al* [10, 11]. However, due to the problems with metastable autoionizing states noted above, single ionization of Ti^{3+} ions was left out of the otherwise very comprehensive investigation. Recently, an experiment on photoionization of Ti^{3+} ions was reported [12] that is closely related to the present study of electron-impact ionization of the same ion.

The conceptually most simple contribution to single ionization of ground-state $Ti^{3+}(3p^6\,3d)$ is the direct removal of one of the outer-shell electrons by a single Coulomb interaction termed *direct ionization* (DI). The threshold energy for removal of the 3d electron is 43.2 eV. At electron energies greater than 77.4 eV the 3p-subshell can also be ionized by a direct process. In addition, indirect processes can lead to the Ti^{4+} product ions observed in the experiments. Excitation of autoionizing states which subsequently decay by electron emission can contribute significantly to the total cross section for net single ionization. Such processes are known in the literature as *excitation–autoionization* (EA). Falk *et al* [3] showed that EA dominates the cross section for single ionization of Ti^{3+}, Zr^{3+} and Hf^{3+} ions by more than a factor of 10 above DI. Common to all these ion species is an excitation of the form

$$n\mathrm{p}^6\, n\mathrm{d} \rightarrow n\mathrm{p}^5\, n\mathrm{d}^2 \tag{1}$$

and subsequent autoionization via a super-Coster–Kronig decay. The oscillator strength for transitions into these autoionizing states is about a factor of 6 higher than that for transitions into the continuum [13].

In addition to EA, resonant processes are possible which lead finally to Ti^{4+} product ions. In such processes, the incident electron is captured into a bound state while an inner-shell target electron is simultaneously excited. The resulting state may have sufficient excitation energy that decay by ejecting two electrons is possible, either by simultaneous emission (*resonant excitation auto double ionization*, *READI*) or by sequential emission via an intermediate state (*resonant excitation double autoionization, REDA*).

The objective of the present experiment was to uncover as many signatures of indirect ionization processes as possible by detailed observation of structures in the energy dependence of the ionization cross section. Another goal was to investigate the unclarified discrepancies between the most advanced theoretical approaches and the only available experimental data obtained previously by Falk *et al* [3].

2. Experiment

A crossed-beams apparatus was employed for the measurements using the well-established animated-beams method for the determination of absolute cross sections [14, 15]. In addition, a high-resolution energy-scan technique [16] was employed to uncover fine details in the energy dependence of the investigated single-ionization cross section. Measurements with energy steps as small as 39 meV were carried out at optimum beam overlap, covering a maximum electron energy range of 110 eV in a single sweep. The statistical precision was improved by increasing the number of sweeps. The resulting relative cross sections were then normalized to absolute cross sections determined by the animated-beams method. The absolute uncertainty of these normalized energy scan cross sections is therefore almost identical to that of the cross sections obtained with the animated-beams method, while the statistical

point-to-point uncertainty can be as low as 0.01% [17]. The apparatus used here has been described previously [18, 19].

In the present experiment Ti^{3+} ions were produced in a Penning discharge ion source operated in sputter mode [20]. After acceleration and magnetic charge/mass analysis, a collimated 36 keV $^{48}Ti^{3+}$ ion beam was crossed with an intense ribbon-shaped electron beam. Typical ion currents in the interaction region were about 1 nA. The Ti^{4+} product ions were separated from the parent Ti^{3+} ion beam with a 90° analysing magnet. After passing through a 180° electrostatic sector field the product ions were counted by a single-particle detector [21] with a detection efficiency of $(97 \pm 3)\%$. The primary ion beam was collected in a movable Faraday cup suitably positioned inside the magnet chamber. The high-current electron gun can be moved mechanically, allowing for translation of the electron beam through the ion beam, which is required for the determination of absolute cross sections with the animated-beams technique. Additionally, this allows for a separate measurement of the background counting rate at a position where there is no overlap of the beams. From separate measurements with the isotope $^{46}Ti^{3+}$ and a comparison of the measured cross sections with those of the most abundant isotope $^{48}Ti^{3+}$, the contamination of the $^{48}Ti^{3+}$ beam with $^{16}O^{+}$ ions was determined to be negligibly small. These measurements were conducted at an electron energy of 900 eV. There the electron gun features an electron current of about 340 mA which, in turn, provides comfortable conditions for absolute cross-section measurements.

A particular experimental feature of the single ionization of Ti^{3+} ions is a huge background count rate due to the presence of ions in autoionizing metastable states [22]. Such states are produced in any ion source in which the electrons are energetic enough to produce triply charged titanium ions in sufficient abundance. When the time of flight from the source to the interaction chamber is of the same order of magnitude as their lifetime, these states decay all along the flight path. This results in detector counts of Ti^{4+} ions without the presence of an electron beam in the interaction region. Hence, very low signal-to-noise ratios were observed in the experiment, especially at low electron energies where the electron current and thus the real signal rate was quite low due to space–charge limited electron beam transport.

Tests with different ion sources were conducted to find suitable conditions for the experiments. In a previous experiment with a 10 GHz electron cyclotron resonance (ECR) ion source [23], background rates as high as 100 kHz nA^{-1} of Ti^{3+} ion current were observed. A bundle of thin 0.5 mm diameter titanium wires mounted on top of a rod was pushed axially to the edge of the ECR plasma and stable beam conditions could be obtained that way. The background level, however, was totally forbidding for crossed-beams measurements. A similar technique of providing Ti atoms to the plasma was tried in a much smaller, less hot, all-permanent-magnet ECR ion source [24] but with very limited success concerning ion currents. Apparently the edge plasma in that source was not sufficiently hot to evaporate Ti from the wires and the plasma was disturbed too much when the wires were pushed in further. In the same source a sputtering mode was tried putting Ti opposite the +10 KV plasma on ground potential such as to accelerate ions onto the Ti surface and sputter Ti atoms, but again, ion currents were in the pA range, too low for the envisaged experiments. Also a titanium metallocene was tried following the prescriptions of Koivisto *et al* [25] but again ion currents were much below 1 nA.

Somewhat better success was obtained by evaporating Ti into the ECR plasma. This was tried with direct-current heated titanium filaments and with an oven mounted inside the ECR plasma chamber. With the heated wire, currents in the nA range were possible, however, stable conditions with sufficient ion current could not be maintained. The wires frequently broke under conditions producing sufficient ion currents. With the evaporation oven, conditions were stable but, given the geometrical limitations set by the plasma chamber, the oven could

not be thermally insulated sufficiently to reach the high titanium boiling point of 1941 K and thus ion currents were again only in the pA range. Moreover, background rates as high as 20 kHz nA^{-1} were observed.

The Penning source provided the lowest level of metastable beam contaminations and hence the least background. Particularly with fresh titanium sputter electrodes, allowing for operation at low discharge power, background levels could be as low as 5 kHz nA^{-1}. Even then, the signal-to-background ratio was only about 1/40 at 100 eV electron energy. Therefore, a voltage-labelling technique was employed to separate the product ions arising from the beam-crossing region from those produced by autoionization or other processes elsewhere along their flight path. An additional voltage of −1500 V was applied to the interaction region for that purpose. Thus all Ti^{4+} ions produced in that region from parent Ti^{3+} ions had a net energy loss in the laboratory frame of 1500 eV compared to those created elsewhere. This energy difference was sufficient to separate the two components of the Ti^{4+} product ion beam in the second analysing magnet and to suppress the background level by about a factor of 8. At an electron energy of 100 eV a signal-to-background ratio of 1/5 was obtained at a maximum counting rate of 2.65 kHz.

The systematic uncertainty of absolute cross sections was carefully estimated at a level consistent with 95% confidence level on statistical uncertainties (two standard deviations). It varies from 9% at 50 eV to 7% for energies greater than 100 eV. Typical total experimental uncertainties at electron energies of 50 eV, 100 eV and 500 eV are 16%, 9% and 7%, respectively. The uncertainty of the electron energy scale is estimated to be less than 1 eV. All energies in this paper are given in the electron–ion centre-of-mass frame.

3. Results

3.1. Overview

Figure 1 presents an overview of the cross section in the energy range from 40 eV to 1000 eV. Also shown are the results of Falk *et al* [3, 4] and the cross section for direct ionization represented by the three-parameter Lotz-formula (solid line) including ionization of the 3s-, 3p- and 3d-subshells [26, 27]. The data indicate that most of the measured cross section results from processes other than DI. The comparison reveals a discrepancy between the present cross-section measurement and the previous data of Falk *et al* amounting to 30% near the cross-section maximum. The present measurements also suggest a bump in the range between 500 eV and 600 eV, but such a feature was absent in fine energy scans covering this region and is not believed to be real.

The measurements indicate significant structures in the cross section at energies below 150 eV. To better highlight the details, the energy range from 40 eV to 150 eV is shown separately in figure 2. There are four obvious steps in the rising slope of the cross section above threshold, namely at 45 eV, 49 eV, 65 eV and 75 eV. An additional step might be present near 56 eV. At the present energy resolution of approximately 0.5 eV, peak features due to resonant ionization processes are not obvious.

Just above the 3d ionization threshold the cross section shows its steepest increase. This feature is associated with indirect processes of the type

$$e + (3p^6\,3d) \rightarrow (3p^5\,3d^2\,{}^2F) + e' \rightarrow (3p^6) + e' + e''. \tag{2}$$

Although an excitation into the configuration $3p^5\,3d\,4s$ is energetically possible above 50 eV, there is a plateau in the measured cross section in that region. The absence of a feature is attributed to a vanishingly small oscillator strength for the transition $3p^6\,3d \rightarrow 3p^5\,3d\,4s$ [13].

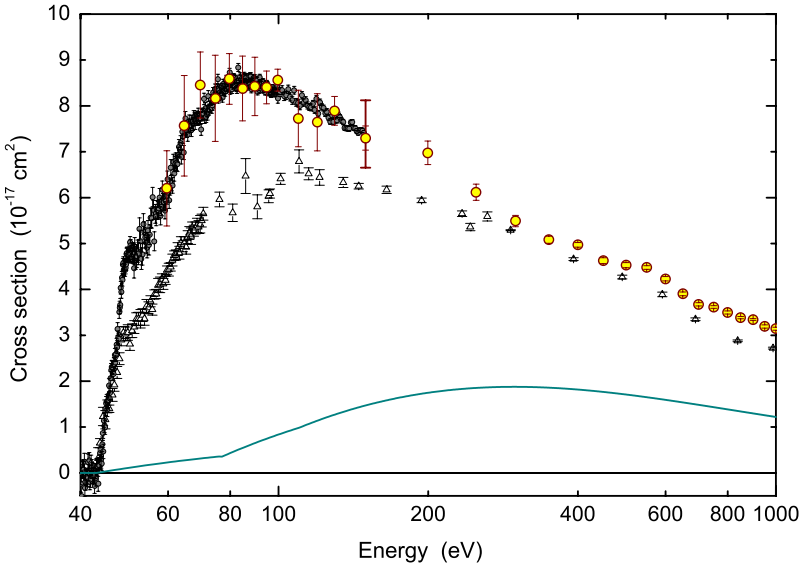

Figure 1. Cross sections for electron-impact single ionization of Ti^{3+} ions: present absolute measurements (open circles); present energy scan data (black dots); measurement of Falk *et al* (open triangles with one-standard-deviation statistical error bars). The contribution of direct ionization (DI) is represented by the Lotz formula (solid line) [27]. For the present measurements statistical uncertainties are shown by the error bars on each data point. The outer error bar on the absolute data point at 150 eV represents the typical total (two standard deviations) uncertainty of the present experiment.

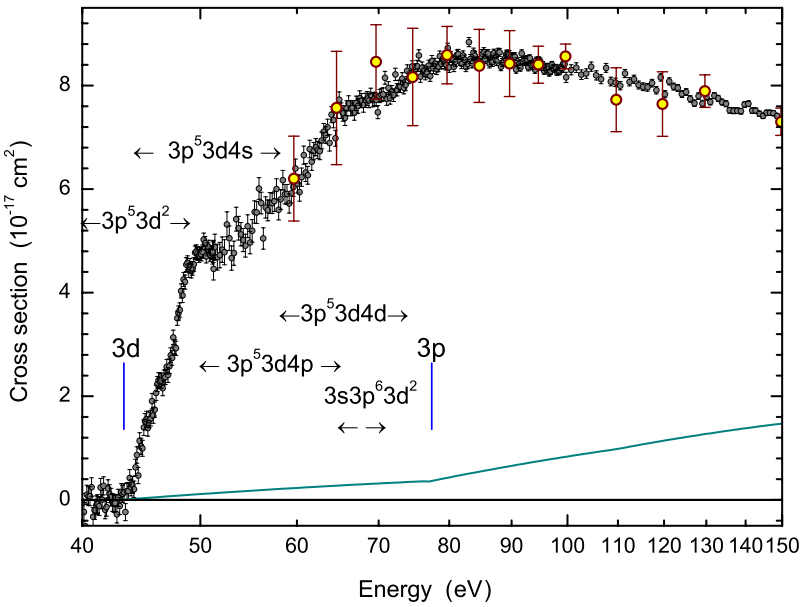

Figure 2. Cross section for single ionization from threshold to 150 eV: present data and Lotz cross section as in figure 1. In addition, energy ranges of states within specified configurations are indicated by horizontal arrows. These energies were determined by employing the atomic-structure code COWAN [28]. The known ionization potentials for the 3d- and the 3p-subshells are marked by vertical bars.

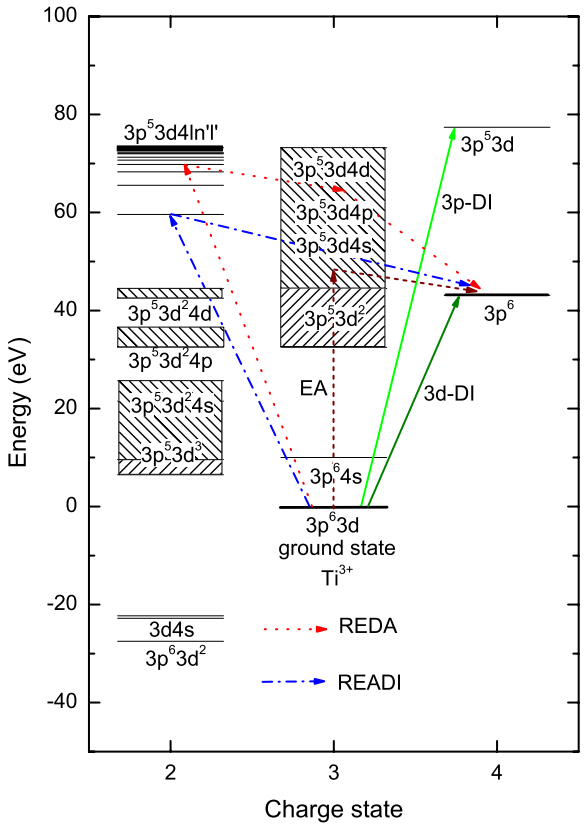

Figure 3. Simplified level scheme of Ti^{2+}, Ti^{3+} and Ti^{4+}. Possible reactions are illustrated by the different arrows. All energy levels are relative to the $Ti^{3+}(3p^6\,3d)$ ground state.

The next excitation that is possible is of a 3p-electron into the 4p-subshell. Here the cross section rapidly increases again up to an energy of about 65 eV. The rise in the cross section above 70 eV is probably due to excitation of a 3s-electron into the 3d-subshell or a 3p-electron into the 4d-subshell. Furthermore, the direct ionization of a 3p-electron becomes possible at energies above 77.4 eV.

Figure 3 shows an energy level diagram of doubly, triply and quadruply charged titanium and illustrates the reaction pathways of processes that can contribute to the observed net single ionization of Ti^{3+}. Energy ranges for several configurations are shown as hatched areas. All energies were calculated by using the COWAN code [28].

3.2. Comparison with theoretical data

Figure 4 shows the present experimental data together with the results of Falk *et al* [3, 4] and the available theoretical calculations [5–7, 9]. The 1991 results of Griffin *et al* [8] (not shown) neglected important contributions to the cross section, and were later corrected by Gorczyca *et al* [9]. For comparison, the three-parameter Lotz cross section is displayed, providing a good estimate of the DI contribution to the observed cross section. As already noted, most of the cross section is due to EA processes. Near threshold, DI is already exceeded by a factor of 20. At low energies, three 3p $\rightarrow$ 3d channels from the $3p^6\,3d$ ground state to states

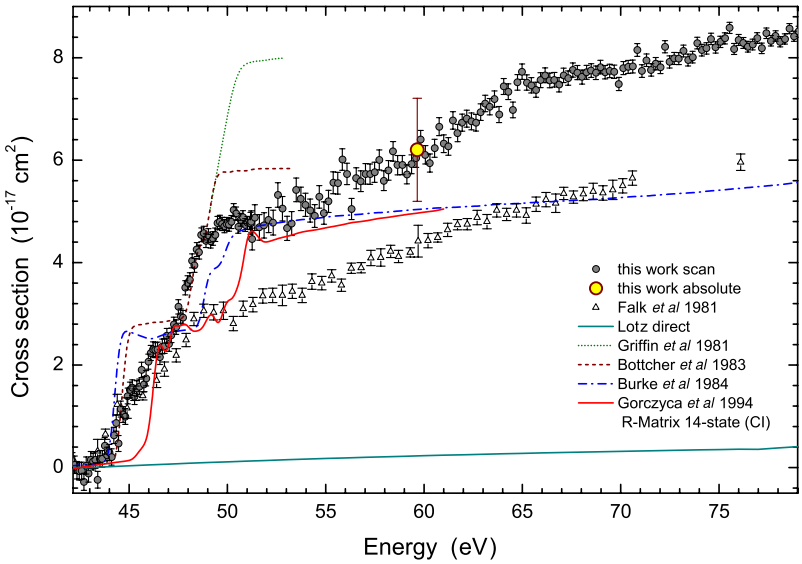

Figure 4. Comparison of the available experimental and theoretical results for single ionization of Ti^{3+} ions. The theoretical *R*-matrix results of Gorczyca *et al* [9] for EA contributions were added to the result of the one-parameter Lotz formula representing DI (see text). All calculations are convoluted with a 0.5 eV FWHM-Gaussian and thus simulate the resolution of the present experiment. Representative total uncertainties of the two absolute measurements are shown for data points near 60 eV. The uncertainties of the present data are given at 95% confidence level, while the data of Falk *et al* show uncertainties at 68% confidence level.

$3p^5(3d^2\,{}^3F)\ {}^2F$, $3p^5(3d^2\,{}^3P)\ {}^2P$ and $3p^5(3d^2\,{}^3F)\ {}^2D$ constitute the dominant indirect channels. This can be attributed to the high oscillator strengths of these transitions [13].

The earliest theoretical description of the total electron-impact single ionization cross section of Ti^{3+} used a Coulomb–Bethe approximation [5]. The theoretical results were about a factor of 2.5 above the experiment of Falk *et al* [3, 4]. In a subsequent study, Bottcher *et al* [6] carried out a full distorted-wave calculation and obtained a 20% reduction with respect to their previous Coulomb–Bethe result, still not explaining the differences with the experiment of Falk *et al*. In 1984 Burke *et al* [7] performed a ten-state *R*-matrix calculation on the ionization of Ti^{3+}. They obtained a value of 4.7×10^{-17} cm^2 at 50 eV, which exceeds the measurement of Falk *et al* but matches the present experimental results very well. Towards higher energies, the calculations of Burke *et al* approach the cross sections measured by Falk *et al*. However, all the ten basis states in this calculation are below 49 eV and thus EA contributions of autoionizing states with higher threshold energies are not included in that first *R*-matrix calculation. Therefore, the EA results of this calculation basically stay at the level of the cross section for exciting states with threshold energies below about 50 eV. Were the calculation to include excitation to states with higher energies, such as $3p \rightarrow 4d$ excitations, then the additional contributions would most probably raise the cross section at higher energies well above the Falk *et al* experiment. The presence of such higher energy contributions is evidenced by the pronounced increase of the present experimental cross section at energies between 65 and 70 eV.

In 1994, Gorczyca *et al* tried a new unified approach to EA [9]. They carried out a 14-state *R*-matrix calculation including configuration interaction (CI). The results were originally added to a distorted-wave calculation of the DI cross section, and convoluted with

a 2.0 eV FWHM-Gaussian to simulate the energy resolution of the Falk *et al* experiment. For comparison with the present experiment the 14-state EA calculation was added to a DI estimate obtained from the one-parameter Lotz formula ($\sigma_{\mathrm{DI}} = 4.5 \times 10^{-14}$ cm$^2/(E \times I) \times \ln(E/I)$, where E is the electron energy and $I = 42.5$ eV the calculated ionization potential of the 3d electron). The sum of EA and DI cross sections was then convoluted with a 0.5 eV FWHM-Gaussian to simulate the energy spread of the present experiment and the result is displayed in figure 4. Again, this calculation did not include excitations 3p $\rightarrow$ nl with $n \geqslant 4$ and hence, the arguments discussed above in connection with the calculation by Burke *et al* also hold here. In principle, these calculations cannot really be compared to experimental cross sections for net single ionization beyond 50 eV, because the experiments contain contributions that are not considered in these calculations. Expanding the basis set of the *R*-matrix calculations to include even only excitations 3p $\rightarrow$ 4l would result in an enormous computational effort.

The comparison shows that all theoretical data are above the measurement of Falk *et al* (at least at energies below 50 eV where they can be expected to be realistic). Apparently, the cross section measurement of Falk *et al* is too low in the region of the cross section maximum. Approximately half of the discrepancy between the two measurements can be accounted for by their combined experimental uncertainties. It is noted that the uncertainties quoted by Falk *et al* are typically only 7% but were estimated at a confidence level of 67%, corresponding to one standard deviation on statistical uncertainties.

While the *R*-matrix calculations agree quite well with the magnitude of the present cross section as far as the step size reached at 50 eV is concerned, there are notable differences between the energy onsets of the different EA contributions in the calculations and the experimental data. Results of a recent photoionization experiment with Ti^{3+} ions [12] shed light on this issue. In that study strong contributions to the photoionization cross section arise from resonant excitation of autoionizing states which then decay by electron emission, as observed in the present work. For the strongest transitions the photoionization experiment provided very accurate excitation energies with uncertainties of only a few meV, except for the very broad $3p^5(3d^2\,{}^3F)\ {}^2F$ resonance which was observed at 43.46(8) eV, straddling the ionization threshold (at 43.267 eV) with a total width of 1.5 eV. In the theoretical analyses by Griffin *et al* and Bottcher *et al* three dominant EA contributions to electron-impact ionization were identified and associated with autoionizing levels $3p^5(3d^2\,{}^3F)\ {}^2F$, $3p^5(3d^2\,{}^3P)\ {}^2P$ and $3p^5(3d^2\,{}^3F)\ {}^2D$. The energies of these levels were calculated to be 44.5 eV, 48.0 eV and 49.1 eV, respectively. In the most recent paper of that group, Gorczyca *et al* [9] performed configuration interaction calculations and found energies for those excitations of 46.29 eV, 50.72 eV and 51.13 eV, respectively. The photoionization experiment by Schippers *et al* resolved even the narrow doublet states and gave quite different energies of 43.46(8) eV for the $3p^5(3d^2\,{}^3F)\ {}^2F$ level, 47.512(1) eV for $3p^5(3d^2\,{}^3P)\ {}^2P_{3/2}$, 47.541(1) eV for $3p^5(3d^2\,{}^3P)\ {}^2P_{1/2}$, and for example, 47.619(1) eV for the $3p^5(3d^2\,{}^3F)\ {}^2D_{5/2}$ level. These energies are in agreement within roughly 0.1 eV with results from plasma spectroscopy by Ryabtsev [29]. They differ from the calculated threshold energies [9] by 2.8 to 3.5 eV, explaining some of the discrepancies between apparent threshold energies in the present electron-impact ionization experiment and the quoted calculations.

In summary, with respect to the magnitudes of the EA features in the cross section, the present measurements are in satisfactory agreement with advanced calculations of electron-impact single ionization of Ti^{3+} ions. The higher energy resolution of the present experiment in combination with spectroscopy results of a recent photoionization experiment provide explanations for the remaining discrepancies between the different theoretical approaches and the new electron-impact data.

Acknowledgment

The support by Deutsche Forschungsgemeinschaft, Bonn-Bad Godesberg, is gratefully acknowledged. The participation of RAP in this project was made possible by a Humboldt Research Award. We thank T W Gorczyca for providing us with the numerical data of the 14-state *R*-matrix results including configuration interaction.

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