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A measurement of the cross section for electron impact ionisation of Fe^+

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Abstract. The cross section for the ionisation process $e + Fe^+ \rightarrow 2e + Fe^{2+}$ has been measured from below threshold up to an electron energy of 750 eV and at energies greater than 25 eV the overall accuracy is estimated to be ±4.3%. The crossed electron–ion beams technique was used and there is evidence that the target ion beam contained a substantial component of metastable ^4D and other long-lived excited Fe^+ ions in addition to the ground-state ^6D ions, but the ionisation data are likely to be directly relevant to Fe^+ ion impurities sputtered from the walls of fusion devices. However, it is probable that the measured cross section is insensitive to the presence of these excited ions, at least at electron energies above about 30 eV. Comparison with theoretically predicted cross sections shows that the McGuire approach is in fair agreement with the experiment but that the parameters proposed by Lotz for his formulation do not yield a satisfactory fit to the measured data.

1. Introduction

The crossed electron–ion beams technique is being used at Culham Laboratory to measure electron impact ionisation cross sections of ions and atoms which are likely to be present as impurities within fusion plasmas. An absolute measurement of the cross section for $e + Fe^+ \rightarrow 2e + Fe^{2+}$ is reported in the present paper.

2. Experimental technique

The crossed-beams apparatus is the same as that described by Montague and Harrison (1983) and the experimental procedure is very similar to that used by these authors for Al^+ ions. Most of the data were obtained using a 2 keV beam of singly charged ^{56}Fe ions with a typical intensity of 2×10^{-9} A although some cross checks were performed using a 4 keV beam. Product Fe^{2+} ions were detected with an efficiency which remained stable within the range 0.68 to 0.66 for the duration of the experiment. At the peak of the cross section the electron beam (typically 150 μA when averaged over the duty cycle of the electron pulses) gave rise to a count rate of typically 340 product ions per second with a 20 to 1 ratio of signal to extraneous ions.

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3. Results and discussions

The cross section for the production of Fe^{2+} ions was measured over the energy range 12 to 750 eV and the results are represented by the experimental points in figure 1. The 90% confidence limits of the counting statistics are smaller than the plotted points. Systematic errors are introduced into the measurement by uncertainties in calibration; the largest of these occur in the detection efficiency of Fe^{2+} ions ($\pm 3\%$) and the effective beam height ($\pm 2\%$). Other systematic errors arise in measurements of the beam currents and they contribute a further $\pm 2\%$. The overall systematic error (compounded in quadrature from the preceding calibration errors) is estimated with 90% confidence to be about $\pm 4\%$. Table 1 lists values of the measured cross section Q taken from a smooth curve drawn through the experimental data points of figure 1. The total error in Q is compounded from the overall systematic error and an error computed from the root mean square of the deviations of the experimental points from the smooth curve.

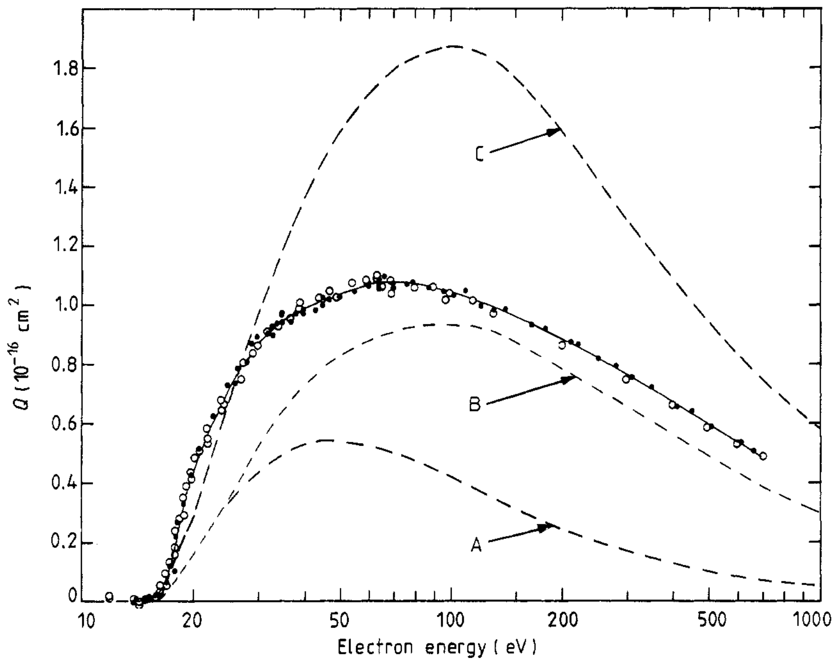

Figure 1. The ionisation cross section of Fe^+ plotted against electron energy. The full and open circles represent data taken with 2 and 4 keV ions respectively. Curve A is the theoretical result of McGuire (1977) using the plane-wave Born approximation for the outer shell only. Curve B is a similar calculation including contributions from the 3d and 3p inner-shell electrons. Curve C is computed from the empirical formula of Lotz (1969).

Near-threshold results for both 2 and 4 keV beams of Fe^+ are shown in figure 2 plotted against the cathode potential V_K. It is apparent for these particular data sets that there is an energy difference of about 1.0 eV in the electron beams. It has been noticed, particularly with beams of high mass ions, that the difference between electron beam energy and cathode potential varies both in time and with energy of the ion beam. The effect is not understood but possible causes are either changes in the contact potential due to contamination produced by sputtering of the shutter used to measure

Table 1. Measured cross section for electron impact ionisation of Fe^+ ions taken from a smooth curve drawn through the experimental points (the full curve in figure 1).

Mean electron energy† E (eV)	Measured cross section $Q(E)$ (10^{-16} cm^2)	Total error‡ in Q (±% of Q)	Mean electron energy† E (eV)	Measured cross section $Q(E)$ (10^{-16} cm^2)	Total error‡ in Q (±% of Q)
14	0.005	60.2			
14.5	0.010	30.3	110	1.029	4.3
15	0.015	20.4	120	1.010	4.3
15.5	0.022	14.3	130	0.993	4.3
16	0.035	57.3	150	0.960	4.3
16.5	0.070	29.0	170	0.926	4.3
17	0.125	16.5	200	0.883	4.3
17.5	0.190	11.3	220	0.854	4.3
18	0.267	8.5	250	0.816	4.3
18.5	0.327	7.4	300	0.761	4.3
19	0.377	6.7	350	0.711	4.3
20	0.465	5.9	400	0.666	4.3
21	0.534	5.6	450	0.625	4.3
22	0.593	5.3	500	0.591	4.3
23	0.647	5.1	550	0.560	4.3
24	0.696	5.0	600	0.532	4.3
25	0.737	4.3	650	0.507	4.3
26	0.775	4.3	700	0.485	4.3
27	0.805	4.3			
28	0.834	4.3			
29	0.857	4.3			
30	0.882	4.3			
32	0.915	4.3			
34	0.936	4.3			
36	0.958	4.3			
38	0.975	4.3			
40	0.989	4.3			
42	1.000	4.3			
45	1.015	4.3			
50	1.039	4.3			
55	1.057	4.3			
60	1.070	4.3			
65	1.077	4.3			
70	1.076	4.3			
75	1.074	4.3			
80	1.070	4.3			
90	1.061	4.3			
100	1.045	4.3			

† ±1.0 eV.

‡ 90% confidence limits. This error is a combination of systematic and random errors.

the profile of the beam currents or changes in the stray magnetic field in the gun region. However the shape of the ionisation onset curve is similar for both ion beam energies and it is characterised by a strong threshold and a weaker threshold some 3 eV lower.

The most probable cause of the lower ionisation threshold is the presence of metastable or long-lived excited ions (lifetime greater than 9 μs) in the Fe^+ ion beam.

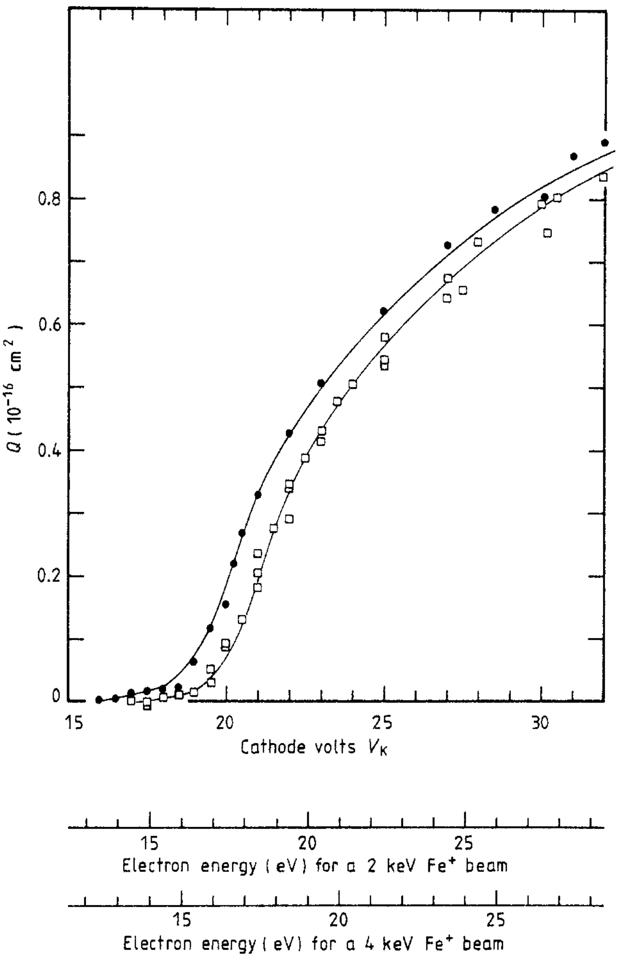

Figure 2. The ionisation signal in the threshold region plotted against the cathode potential V_K of the electron gun for 2 keV (full circles) and 4 keV (open squares) beams of Fe^+.

Ground state Fe^+ has even parity and there are a large number of low-lying states of Fe^+ which also have even parity and which are therefore metastable and have long lifetimes.

Ion production in the sputter source used in this experiment is dominated by electron collisions whereas ion neutralisation in the source is dominated by ion–wall collisions rather than by electron–ion collisions. The wall collision rate will be independent of the excited state of the ion and so the distribution of excited states amongst the Fe^+ ions in the source is likely to be strongly influenced by the relative magnitudes of their ionisation probabilities from the $(3d^6 4s^2)^5D$ ground-state atoms. If it is accepted that the probability for ionisation is greatest to Fe^+ states which are formed without rearrangement of the electron configuration, then the most likely excited state of Fe^+ is the metastable $(3d^6 4s)^4D$ which is formed by outer-shell ionisation of the Fe ground state. There might also be a smaller population of the higher lying quartet and doublet states of this electron configuration (e.g. ^4P, ^4F, etc). Inner-shell ionisation of ground-state Fe could give rise to the $(3d^5 4s^2)^6S$ metastable state of Fe^+ but rearrangement collisions which form states with the $3d^7$ configuration are much less likely. On the basis of these arguments it is to be expected that there will be a large population of ^4D Fe^+ ions in the beam (possibly almost as many as ground-state ^6D). There should also be smaller populations of ^4P and ^4F and, because the electron energy distribution in the ion source extends up to about 40 eV, there may also be a small component of ^6S.

Analogous consideration of the most likely state of Fe^{2+} formed by electron beam collisions with this mixed-state Fe^+ beam (a simplified energy diagram is presented in figure 3) leads to the conclusion that the dominant ionisation channels must be

$$(3d^64s)^6D \rightarrow (3d^6)^5D + e \quad \text{(threshold 16.18 eV)}$$

and

$$(3d^64s)^4D \rightarrow (3d^6)^5D + e \quad \text{(threshold 15.20 eV)}.$$

The spread in electron beam energy (typically 0.6 eV FWHM) coupled to the spread of the energy levels of the ^6D and ^4D states (due to fine-structure levels) precludes identification of the linear slope region due to ionisation of ^4D so that the concentration of this metastable level cannot be determined directly from the data.

Ionisation of Fe^+ observed below the 15.20 eV threshold of the ^4D state probably arises from ^4P and other states of the $3d^64s$ configuration because, at low energy, ionisation of ^6S is only likely to produce Fe^{2+} in ^7S and ^5S states with thresholds of 17.02 and 18.37 eV. This interpretation leads to the assignment of an effective contact potential of −2.6 V for the 2 keV beam data and −3.6 V for the 4 keV beam data and these adjustments have been applied to the data presented in figure 1 and listed in table 1.

At higher electron energies ($E > 20$ eV) it is to be expected that ejection of one of the six inner 3d electrons of Fe^+ will contribute to ionisation. Very many final

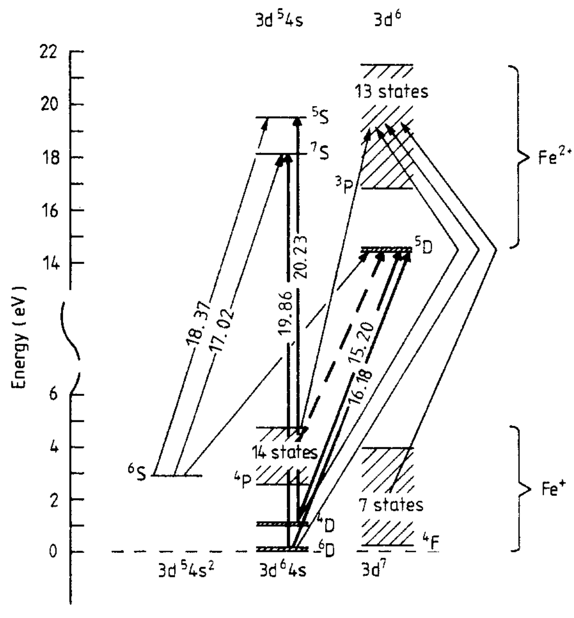

Figure 3. Simplified energy level diagram of Fe^+ and Fe^{2+} showing the transitions considered in interpretations of threshold data. The heavy lines show the most likely transitions.

states are possible but the processes with the lowest threshold energies are

$$(3d^6 4s)^6D \rightarrow (3d^5 4s)^7S + e \quad \text{(threshold 19.86 eV)}$$

and

$$(3d^6 4s)^4D \rightarrow (3d^5 4s)^5S + e \quad \text{(threshold 20.23 eV)}.$$

The present data do not provide clear evidence of thresholds in this energy region. However, in figure 1 it is seen that the estimate of the inner-shell ionisation cross section by means of McGuire's formulation shows that the 3d contribution only rises slowly from threshold. There is some scatter of the experimental points that confuses the issue but it is also possible that the onset of the outer-shell ionisation channels for ^6S at 17.02 and 18.37 eV and ionisation of ^6D and ^4D to higher states of Fe^{2+} with $3d^6$ configuration may obscure the inner-shell thresholds of ^6D and ^4D (see figure 3).

The similarity of the transitions involved and the approximate equality of the transition energies, at least for the ^6D and ^4D levels of Fe^+, signifies that the cross sections for production of Fe^{2+} from these levels are likely to be similar in magnitude and energy dependence. It can therefore be concluded that the presence of a substantial concentration of ^4D ions in the ground-state beam will not have much influence on the measured cross section at energies in excess of about 30 eV. There can be few practical situations where Fe^+ ions occur solely in the ground state and in particular the distribution of excited states produced in the sputter ion source is expected to be similar to those associated with sputtering erosion in the boundary of a fusion plasma. Thus the present data directly reflect the needs of fusion research.

In view of the expected insensitivity to excited components of the Fe^+ beam, the measured data are compared with predicted cross sections for ionisation from the ground state. In figure 1 curve A is the outer-shell and curve B the outer-plus-inner-shell ionisation cross sections calculated using McGuire's (1977) scaled cross section of atomic subshells. An alternative calculation in which ^6D and ^4D ions are taken in the ratio 3:2 yields a total cross section which is within 5% of that shown (curve B) for the ^6D contribution only. There is a growing body of evidence that the McGuire approach underestimates the cross section at low energies (less than twice threshold) but in this particular case the magnitude at higher energies also appears to be low. Curve C shows a calculation using the Lotz (1969) formula for 4s, 3d and 3p subshells. Both the excessive magnitude of the cross section and the shift of the peak to high energy appear to be characteristic of the applications of the Lotz parameters to the limited number of complex singly charged ions studied to date.

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