X-ray observations of helium-like scandium from the Alcator C-Mod tokamak

J E Ricet, M A Graff, J L Terry, E S Marmar, K Giesing and F Bombardat
† Plasma Fusion Center, MIT, 175 Albany St, Cambridge, MA, 02139-4307, USA
‡ Associazione ENEA-Euratom per la Fusione, CP 65, 00044, Frascati, Italy

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Abstract. Scandium (Z = 21) has been injected into the Alcator C-Mod tokamak. X-ray wavelengths of Δn = 1 transitions to the ground state in ScL9+ and ScL8+ have been accurately determined. Time-resolved spectra have been obtained from different radial locations following the injections and have been compared with favourable agreement to the results of collisional radiative-transport code modelling. X-rays emitted from the outermost regions of the plasma (r/aL ≥ 5) appear in time after x-ray emission from the plasma centre. These x-rays arise from upper levels in ScL9+ populated by radiative recombination of Sc20+, which can only exist in the outer regions after the scandium has penetrated to the plasma centre, become ionized to ScL8+, and diffused back out before recombining. The density of scandium in the plasma has been determined for a variety of operating conditions. Only about 10% of the injected scandium penetrates to the plasma centre, and the scandium density in the plasma decreases with increasing electron density.

1. Introduction

There is considerable interest in the x-ray emission from helium-like ions from tokamak plasmas [1–8], for comparison with atomic structure calculations, for measurement of ion and electron temperatures and for determination of ionization balance. Most of these spectrally resolved observations are taken along centrally viewing chords so the effects of the nearly universal anomalous impurity transport are not apparent. There are some observations from the plasma edge [9] which demonstrate the substantial effects of impurity transport on x-ray spectra, but these are all for steady state conditions. There are several spaces and time-resolved measurements of x-ray emission from impurity injection experiments [10, 11] but these are from x-ray diode arrays with no spectral resolution. In this paper we present the first spectrally, spatially and temporally resolved x-ray measurements of impurity injections into tokamak plasmas.

Scandium has been injected into the Alcator C-Mod tokamak [12] using the laser blow-off technique [13], in order to study impurity transport [10, 11, 14–17]. A typical deuterium discharge into which scandium was injected is depicted in figure 1. Plasma parameters at the injection time of 0.550 s were BT = 5.2 T, Ip = 0.85 MA, elongation = 1.6, Te = 1600 eV, ne = 1.6 × 1020 m−3 and the minor radius on the midplane = 22.5 cm. The nominal major radius (magnetic axis) of the plasma was 69.0 cm. Effects of the injection can be seen on the total radiated power, the central soft x-ray trace and Zeff. One of the diagnostics used to observe the injected scandium was a 5 chord, independently scannable high-energy resolution crystal x-ray spectrometer array [18]. The time history from one of the crystal spectrometers viewing the plasma centre is shown in figure 1. A spectrum of the central
Figure 1. The time histories of several parameters of interest for a discharge into which scandium was injected. (A description of the various diagnostics from which these traces were obtained can be found in [12].)

Figure 2. The $\Delta n = 1$ spectrum of helium-like Sc$^{19+}$. 
scandium x-ray emission is shown in figure 2. The spectrum is dominated by the resonance line (w). The intercombination (x, y) and forbidden (z) lines, as well as some satellites (s, q, r, k, j), are visible.

Figure 3. 5p-, 6p-, 7p- and 8p-1s transitions in hydrogen-like Ar$^{17+}$.

Table 1. The $\Delta n = 1$ transitions of Sc$^{19+}$ and Sc$^{18+}$. The measured wavelengths are given in the fourth column. In the last column are the theoretical wavelengths of helium-like scandium from Vainshtein and Safronova [24]. In the penultimate column are theoretical wavelengths for helium-like scandium and the satellites with the spectator electron in the $n = 2$ level from Vainshtein and Safronova [21], an $n = 3$ spectator satellite from Vainshtein and Safronova [22] and a beryllium-like satellite from Boiko et al. [23].

| Name | Transition | Rel. int. | $\lambda$ (mÅ) | $\lambda$ [21–23] | $\lambda$ [24] |
|------|------------|-----------|----------------|----------------|----------------|
| w    | 1s2p $^1P_1$-1s$^2$ 1S0 | 1.000     | 2873.1         | 2872.3         | 2873.2         |
| 4    | 1s2p4p-1s$^2$4P | 0.065     | 2875.0         | —              | —              |
| 3    | 1s2p3p $^2P_{3/2}$-1s$^2$3p $^2P_{3/2}$ | 0.064     | 2877.7         | 2876.2         | —              |
| x    | 1s2p $^2P_2$-1s$^2$ 1S0 | 0.103     | 2883.2         | 2882.4         | 2883.3         |
| s    | 1s2s2p $^2P_{3/2}$-1s$^2$2s $^2S_{1/2}$ | 0.056     | 2884.9         | 2883.8         | —              |
| y    | 1s2p $^3P_1$-1s$^2$ 1S0 | 0.154     | 2887.0         | 2886.1         | 2887.0         |
| q    | 1s2s2p $^2P_{3/2}$-1s$^2$2s $^2S_{1/2}$ | 0.049     | 2893.2         | 2892.4         | —              |
| r    | 1s2s2p $^2P_{1/2}$-1s$^2$2s $^2S_{1/2}$ | 0.032     | 2895.7         | 2895.2         | —              |
| k    | 1s2p $^2D_{3/2}$-1s$^2$2p $^2P_{1/2}$ | 0.043     | 2898.2         | 2897.4         | —              |
| j    | 1s2p $^2D_{5/2}$-1s$^2$2p $^2P_{3/2}$ | 0.030     | 2901.2         | 2901.0         | —              |
| z    | 1s2p $^3S_1$-1s$^2$ 1S0 | 0.224     | 2902.8         | 2902.2         | 2903.0         |
| $\beta$ | 1s2s2p $^1P_1$-1s$^2$2s $^1S_0$ | 0.028     | 2911.5         | 2910.7         | —              |
| —    | 1s2s2p $^4P_{3/2}$-1s$^2$2s $^2S_{1/2}$ | 0.025     | 2915.7         | 2914.4         | —              |

2. Wavelength determination

In order to identify all of the transitions in this spectrum, and to accurately determine the wavelengths, advantage has been taken of the occurrence of several high-$n$ transitions of
hydrogen-like argon in this same spectral range. In particular the 5p-, 6p-, 7p- and 8p-1s lines with precisely known wavelengths of 2917.50 mA, 2881.04 mA, 2859.38 mA and 2845.51 mA, respectively [19], have been used to calibrate the dispersion of the spectrometer [20]. Argon was puffed into the early phase of the discharge using a piezo-electric valve; a spectrum of these Ar$^{17+}$ lines is shown in figure 3. For scandium, line identifications, relative intensities and measured wavelengths, along with calculated wavelengths [21–24] are given in table 1. The measured wavelengths are accurate to ±0.1 mA. The wavelengths from [24] are in excellent agreement for the helium-like lines, but there is a systematic shift of about 0.8 mA for all of the transitions of [21–23], because QED effects were not taken into account.

3. Synthetic spectra

A collisional-radiative model for the emissivities of helium-like ions [25, 26] has been used in conjunction with the impurity transport code MIST [27] in order to calculate the chord brightness profiles of the lines in the Sc$^{19+}$ spectrum. The $n = 2$ levels in helium-like scandium are populated by collisional excitation of the helium-like state, inner-shell ionization of the lithium-like state, and radiative and dielectronic recombination of the hydrogen-like state. Appropriate coefficients have been interpolated from the tables of [25]. For the $n = 2$ and 3 dielectronic satellites, the values of the intensity factor ‘g’ have been taken from [21, 22]. For the inner-shell satellites, excitation rates have been interpolated from the rates for lithium-like calcium [28] and titanium [29]. This allows for calculation of the emissivity profiles of all of the lines in the spectrum, given charge state density profiles and measured electron density and temperature profiles. The charge state density profiles are taken from MIST calculations, where the impurity transport is modelled typically with a spatially constant diffusion coefficient and with no convective velocity ($v = 0$). Electron temperature and density profiles for the discharge of figure 1 are shown in figure 4, which were taken from ECE [30] (electron cyclotron emission) and laser interferometer [31] measurements, respectively.

![Figure 4](image_url)
Emissivity profiles of all the lines have been calculated for a case with the plasma parameters of the shot shown in figure 1, and with a diffusion coefficient of 5000 cm² s⁻¹, consistent with a 1/e decay time of 19 ms for central brightness time histories. The emissivities (and charge state densities) are taken to be constant along each flux surface (reconstructed from the FETT [32] code), and brightnesses corresponding to the actual spectrometer lines of sight are then calculated. From these brightnesses, synthetic spectra are then constructed, with the wavelengths of the helium-like lines taken from [24], and with the satellites of [21,22] shifted by 0.8 mA towards the red. Appropriate line widths from measured ion temperatures and instrumental widths are also employed. An example is shown in figure 5, for a total of 5 × 10¹⁷ injected scandium atoms, to be compared with the spectrum of figure 2. In this case the brightnesses were integrated over the entire time the scandium was in the plasma. The satellites with n > 3 spectators, and those with wavelengths longer than 2905 mA have not been included. The agreement between the synthetic and observed spectrum is good, supportive of the collisional-radiative model, the transport coefficients and the observed electron temperature profile.

4. Spatial and temporal variations

Since there are five spectrometers viewing along different chords in the plasma, spatial information about the Sc¹⁹⁺ brightness profiles is available for these injections. Shown in figure 6 are the five spectrometer lines of sight superimposed on the flux surface reconstructions for a particular discharge. The origin of the coordinate system used to describe the spectrometer views is the nominal centre of the machine, located at Z = 0 and R = 67.0 cm, indicated by an ‘X’. The magnetic axis of this discharge at the time of the injection (0.8 s) was at Z = −1.9 cm and R = 69.0 cm, and is indicated by a ‘+’ symbol. In the lower right-hand corner the vertical locations are listed (in metres) where the five lines of sight intersect the vertical plane at R = 67.0 cm. Just to the left of these numbers are listed the radii of the innermost flux surfaces (mapped onto the magnetic horizontal
midplane on the outer half of the plasma) that the spectrometer lines of sight intersect (are
tangent to). These locations are indicated on the magnetic midplane by a different symbol
for each spectrometer. For example, the spectrometer 5 line of sight intersects the vacuum
vessel centre vertical plane ($R = 67.0$ cm) at 16.0 cm above the centre ($Z = +16.0$ cm).
The innermost flux surface that this line of sight intersects can be traced back to $R = 82.7$
cm on the magnetic midplane ($Z = -1.9$ cm), which is indicated by a square.

Shown in figure 7 by the narrow curve is a spectrum taken along a line of sight which
crosses the $R = 67.0$ cm vertical plane 12.7 cm below the midplane ($R = 77.3$ cm), for a
discharge similar to that shown in figure 1. The highest electron temperature along this chord
for this discharge was around 1200 eV. Notice that the intensities of the intercombination
and forbidden lines, as well as the satellites, have grown relative to the resonance line,
compared to figure 1, since the electron temperature is lower. Shown in figure 7 by the
heavy curve is a synthetic spectrum calculated for the line of sight of the observed spectrum.
Again, the agreement between the observed and calculated spectra is quite good. In fact this
situation persists out to at least 80% of the minor radius. Shown in figure 8 by the narrow
curve is a spectrum taken from along a line of sight 18.3 cm above the midplane ($R = 83.8$
cm), where the maximum electron temperature was around 600 eV. Although the signal
level is very low, it is clear that the forbidden line intensity is greater than or equal to that
of the resonance line, indicative of a recombining plasma [9]. At this radius, the contribution
from radiative recombination to the population of the upper level for the forbidden line is
a factor of three larger than from collisional excitation. Also in figure 8 the corresponding
synthetic spectrum (heavy curve) is shown, again with fairly good qualitative agreement.
There are no measurements at major radii larger than this because the signal level is too low.
In figure 9 we show the ratios of the forbidden line $z$, the inner-shell satellite $q$ and the dielectronic satellite $k$ to the resonance line $w$ taken along four lines of sight. The horizontal axis is the major radius on the plasma midplane of the innermost flux surface to which the individual line of sight is a tangent. These lines, as well as all lines in the spectrum, increase relative to the resonance line with increasing distance away from the plasma centre, at least out to 84 cm ($r/a = 0.8$), in accordance with a drop in the electron temperature. The curves are the ratios from the calculated brightness profiles, and are in good agreement.

All of the results discussed above are based on spectra integrated over the duration of
Figure 9. Observed (symbols) and calculated (curves) line ratios of $z/w$, $q/w$ and $k/w$ versus major radius. Typical error bars are shown.

Figure 10. Observed time histories of scandium injection along chords at (a) +3.0 cm, (b) -12.7 cm and (c) +18.3 cm, with code predictions (smooth curve). The injection time was 0.550 s.

The injections. Temporal information is also available from the spectrometer array. Shown in figure 10 are the time histories of three total spectrometer signals, integrated over the wavelength region between 2.86 and 2.94 Å as functions of time. In this case the injection time was 0.550 s. The three traces were from spectrometers looking at +3.0, -12.7 and +18.3 cm, respectively. The signals all decay with a 1/e time of about 19 ms, which implies a diffusion coefficient of about 5000 cm$^2$ s$^{-1}$. Notice that the signal at -12.7 cm (b) rises to a peak in about 5 ms, nearly a factor of 2 faster than the more central chord (a). The signals at these radii are dominated by lines populated by collisional excitation of helium-like scandium, which exists over most of the plasma. During the influx phase of the injection, it takes longer for the scandium to reach the plasma centre, so the signal shown in
Figure 11. The ratios of the brightnesses at −9.4 cm of several satellites to the resonance line at two different times during an injection, the first 25 ms and the last 50 ms. '3' represents the satellites with \( n = 3 \) spectators at 2877.7 mA.

(a) peaks later than the signal in (b). However, the outermost signal at 18.3 cm (c) actually peaks later than that of the central chord. This is because, at these extreme radii, the upper levels for the lines are mainly populated by radiative recombination of hydrogen-like Sc\(^{20+}\) and during the influx phase of the injection, there is no hydrogen-like scandium at this radius. So it is only late in the injection, after Sc\(^{20+}\) is born at the centre of the discharge and then diffuses out to this radius, that the signal appears. Also shown (by the smooth curves) are the code results, which are in excellent agreement.

There is also spectral information available as a function of time. For all of these injections, spectra were collected with 50 ms integration time during the discharges, and although these injections were relatively fast (a typical total duration was 80 ms), at least two spectra were collected per injection. For the spectrometer looking at −9.4 cm (\( R = 74.2 \) cm), differences were seen in the first 25 ms 'ionization' phase of the injections and the last 50 ms 'decay' phase. In particular, the inner-shell satellites were all stronger relative to the resonance line during the rise phase. The upper levels of these inner-shell satellites are mainly populated by excitation of lithium-like Sc\(^{18+}\). Shown in figure 11 are the ratios of several satellites to the resonance line during the rise phase (left edges of the lines) and the decay phase (right edges). The satellites q and r are brighter during the early phase due to a greater abundance of Sc\(^{18+}\) at this time. This point is supported by the code modelling.

In order to emphasize this, and to explain quantitatively the later peaking of the total line brightness time history at the outermost chord, brightness time histories of the individual lines have been calculated. Time histories for q, w and z for the line of sight 18.3 cm above the midplane (\( R = 83.8 \) cm) are shown in figure 12. Each line demonstrates the dominance of a different charge state in the population of the upper level, for q the lithium-like stage, for w helium-like, and for z hydrogen-like. These three charge states appear at this radius sequentially in time, the Li-like as the scandium diffuses into the centre and the H-like as the scandium leaves the plasma. The total spectrometer time history (as in figure 10) is the sum of all lines in the spectrum and since the forbidden line dominates the spectrum at this radius, the total signal peaks late in time, after the peak along the central chord. This
is corroborated in figure 13 which shows the calculated charge state density profiles for lithium-like (18+), helium-like (19+) and hydrogen-like (20+) scandium at three different times after the injection. Shown by the dotted curves are the profiles at 1.7 ms, by the full curves the profiles at 4.2 ms and by the broken curves the profiles at 25 ms. At R = 84 cm, the lithium-like state has the highest density at 1.7 ms. At 4.2 ms at this radius, the helium-like state dominates. At the latest time shown, 25 ms, the hydrogen-like scandium density is at its highest relative to the helium-like density. Since radiative recombination overwhelmingly dominates the population of the triplet levels of Sc^{19+} at the electron temperature of this radius, this amount of Sc^{20+} allows the forbidden line, \( z \), to dominate
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Figure 14. Calculated spectra for a chord viewing 18.3 cm above the midplane ($R = 83.8$ cm) for three different times after the injection, (a) 0–3.4 ms, (b) 3.6–6.6 ms and (c) 11.6–48.5 ms.

the spectrum [9]. Synthetic spectra at three different times for this view ($R = 83.8$ cm) are shown in figure 14. In figure 14(a), from 0–3.4 ms (the ionizing phase of the injection), the inner-shell satellites are the strongest lines in the spectrum. From 3.6–6.6 ms (figure 14(b)), the resonance line is strongest and in figure 14(c), from 11.6–48.5 ms, the forbidden line is dominant (the recombining phase).

5. Scandium density estimates

The absolute sensitivities of the spectrometers have been calculated from geometric factors, crystal reflectivities, window transmissions and detector sensitivities. (Impurity densities for argon, for example, determined from line brightnesses are in agreement with densities determined by two independent methods, namely from the x-ray pulse height analyser and from rises in $Z_{\text{eff}}$ during argon puffing.) From scandium line brightnesses, the scandium density during an injection can be determined from knowledge of the electron density and temperature profiles, line population modelling and charge state profiles. For the discharge of figure 1, the deduced central scandium density at the peak of the injection was $6 \times 10^{10}$ cm$^{-3}$, yielding a contribution to $Z_{\text{eff}}$ of 0.13. This is consistent with a measured rise in $Z_{\text{eff}}$ from visible bremsstrahlung of 0.12. Typically, $5 \times 10^{17}$ atoms are injected at the edge, implying, for a plasma volume of 0.92 m$^3$, that at least 10% of the scandium is reaching the plasma core. This is a considerably larger percentage of penetration than observed for argon introduced at room temperature through a gas valve.

Similar amounts of scandium were injected into a variety of plasma conditions. In particular, a series of discharges were taken varying the electron density with constant plasma current (850 kA) and toroidal magnetic field (5.2 T). Shown in figure 15 is the deduced scandium density as a function of central electron density for this series of plasmas. For all of these data points, the different electron density and temperature profiles, and corresponding changes in the charge state balance, have been taken into account. At the higher electron densities, less scandium is actually reaching the centre, indicating a possible screening effect due to changes in the edge conditions. In discharges with higher central electron densities, the edge electron densities were also higher. The measured transport
coefficients were unchanged during this density scan. Intrinsic impurity densities in the plasma are also lower at higher electron densities.

6. Conclusions

Scandium has been injected into Alcator C-Mod plasmas. Accurate x-ray wavelengths of $\Delta n = 1$ ground-state transitions in Sc$^{19+}$ and Sc$^{18+}$ have been determined. Spectra have been obtained from various locations in the plasma and upper levels are populated by excitation and dielectronic recombination over most of the plasma volume and by radiative recombination in the edge regions. Observed spectra and brightness time histories are in good agreement with synthetic spectra and time histories calculated from a model which includes anomalous impurity transport, observed electron density and temperature profiles and collisional-radiative line emissivities. Absolute scandium densities have been determined for a variety of conditions. In a typical case, about 10% of the injected scandium penetrates the plasma edge to reach the centre and less injected scandium penetrates to the core as the electron density is increased.

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