Observation of O V visible transitions in a tokamak divertor plasma

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We report the observation of two unusually bright, visible lines from Be I–like oxygen, an impurity intrinsic to tokamak plasmas. Collisional-radiative (CR) models using detailed atomic structure are used to predict line brightnesses in agreement with observations. Because the O V ion exists in the divertor region of a tokamak, and since visible transitions can be easily measured, these lines can serve as a useful diagnostic of impurity concentration and ion temperature in a region of the plasma crucial to impurity control and energy balance.

The passively observed visible spectra of an impurity in a tokamak discharge has largely been used as a measure of the source rate and ion temperature of the impurity in the extreme edge of the plasma, near the material surfaces with which it is in contact [1]. It has been presumed that in the typical edge plasma of present devices ($T_e < 150$ eV, $n_e < 10^{14}$ cm^{-3}), visible line radiation will be emitted only from the lowest few ionization states of the impurity in the extreme edge ($T_e < 50$ eV), since at higher electron temperatures ($50 < T_e < 150$ eV) away from the surface the ions will undergo multiple ionization, and the only visible transitions from these multiply charged ions will be between upper levels which are weakly populated in low density ($n_e < 10^{14}$ cm^{-3}) plasmas. Thus among plasma physicists, the spectroscopic study of plasmas at $T_e > 50$ eV has been confined to the ultraviolet domain. Since most ultraviolet measurements need to be made *in vaccuo,* the measurements of such plasmas are limited. For example, in magnetic fusion research, there is much interest in the region of a tokamak plasma near the so-called magnetic separatrix of a poloidal divertor at electron temperature T_e of about 100 eV [2]. But the poloidal divertor topology presents a diagnostic challenge since this critical part of the plasma is highly poloidally asymmetric, and ultraviolet diagnostics are usually limited to one viewing chord. Conversely, in the visible, multiple views can more easily be obtained using optical fibers. Thus if suitable visible lines could be found in this part of the plasma, they could potentially be useful as an impurity-based plasma diagnostic.

Oxygen is a contaminant in almost all laboratory plasmas, and its potential as an ultraviolet spectroscopic diagnostic of both electron density and temperature has been developed over the past decade [3,4]. The collisional-radiative (CR) models upon which most previous work is based include only the lowest 10 or 20 energy levels, thus excluding all or most of the $\Delta n = 0$ ($3 \rightarrow 3$) and ($4 \rightarrow 4$) transitions. Since in Be I–like oxygen (ionization potential $V_{\text{pot}} = 113.9$ eV) visible radiation will exist only for $\Delta n = 0$ transitions within the $n = 3$ and $n = 4$ energy levels, CR models to date (for oxygen and other Be I–like ions similar in Z) have not contained information necessary to study these systems.

The energy-level structure of the O V ion had been reported on by Bockasten and Johansson [5]. They studied θ-pinch discharges with high resolution spectrometers in the 340–7700 Å range. They deduced the level structure from the resulting spectra, and determined 132 energy levels. Since their plasmas were dense compared to a tokamak plasma, the intensities of the lines they measured are not meaningful with regard to the latter. As will be seen shortly in this paper, two of the lines in the visible that they listed are quite bright in a typical tokamak plasma. Without a CR model, however, these lines could at most indicate the presence of O V, and without an understanding of how these lines could be so bright, these lines have been largely ignored in experimental spectra. This situation has begun to be remedied by the adoption of the Hebrew University–Lawrence Livermore Atomic Codes (HULLAC) to the study of the first $4n$ shells of medium-Z (C–Ar) Be I–like ions. HULLAC has been used to construct a 98-level CR model for the O V ion and predicts a pair of bright visible lines from this ion. These lines were then easily found in a typical tokamak spectra from the DIII-D device, and a search of the literature shows that these levels are among those determined by Bockasten and Johansson. This paper presents *ab initio* calculations for transitions previously mentioned in the spectroscopic literature, and demonstrates their existence in a real plasma. Also, a preliminary consideration of their diagnostic potential is given.

The *ab initio* atomic structure data for berylliumlike charge states (ground state $1s^2 2s^2$) of intermediate-Z elements has been generated using the HULLAC package [6,7]. We have identified the LS states of the O V system using published energy-level values [8]. CR models were constructed by using electron impact excitation rates generated by CROSS [9]. To account for possible resonances in the collisional excitation rates, we have taken the R-matrix collisional excitation rates of Berrington *et al.* [10] for all transitions between the ten energy levels of the six lowest LS-target states: $2s^2\ {}^1S$, $2s2p\ {}^3P^o$, ${}^1P^o$, $2p^2\ {}^3P$, ${}^1D$, and ${}^1S$.

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Line emissivities for the transitions studied were found by multiplying the total radiative decay rate from a given level by the population in that level. The steady state coronal population for each level was found by solving the set of equations

$$N_j \left[\sum_{i<j}^{M} (A_{ij} + n_e Q_{ij}) + \sum_{k>j}^{M} n_e Q_{kj} \right]$$
$$= \sum_{k>j}^{M} N_k (A_{jk} + n_e Q_{jk}) + \sum_{i<j}^{M} N_i n_e Q_{ji} ,$$

where N_j is the population of level j, A_{ij} is the radiative decay rate from level j to level i, Q_{ij} is the collisional-rate coefficient in $cm^3 sec^{-1}$ from level j to level i for excitation or de-excitation, and M is the number of energy levels ($M=98$) in the model for a given ion. Figure 1 shows the energy-level structure for the $2p3l$ ($l=s,p,d$) configurations in O V. The levels are grouped by LS multiplet. The energy units on the vertical axis are not to scale and provide a rough idea of where these levels occur. Written in bold above each multiplet in Fig. 1 is the sum of the steady state populations at $T_e = 50$ eV and $n_e = 1 \times 10^{13}$ cm^{-3} of each level in the multiplet. The levels of the $2p3d$ ^3F multiplet are found to have population orders of magnitude greater than the populations in other nearby LS multiplets. The reason for this will be explained below.

We compared out CR models to results published by Finkenthal et al. [3] for the ratio of the $2s2p$ $^3P - 2p^2$ ^3P emission to the $2s^2$ $^1S - 2s2p$ ^1P emission. This ratio depends strongly on the collision rates between the ten energy levels of the six lowest LS-target states. We found that for a temperature near the predicted ionization equilibrium temperature, our model yielded a value of $R = 0.65$ without the R-matrix rates, and a value of $R = 0.89$ with the R-matrix rates for collisional transitions between the ten lowest energy levels. The calculated R-matrix value at the same temperature published in
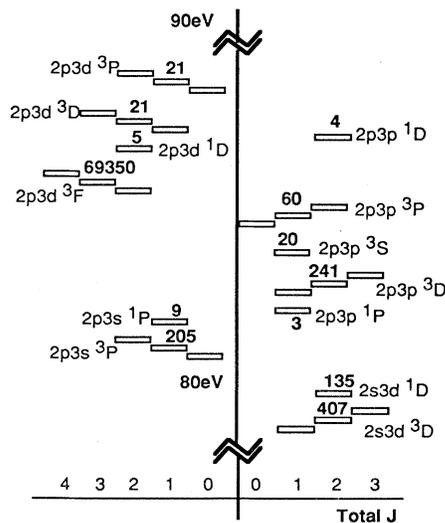
Ref. [3] is near 0.96 (see Fig. 3b in Ref. [3]).

An artifact of our intermediate coupling calculation is that the configuration interaction allows what would be ordinarily LS-forbidden transitions to take place. Further, our models included all radiative decay channels for electric and magnetic dipole and quadrupole ($E1$, $M1$, $E2$, and $M2$, respectively) transitions, creating many more channels for population flux between levels. While the effects of both the configuration interaction and the higher multipole transitions will be small on the overall kinetics of the $\Delta n = 0$ ($3 \rightarrow 3$) berylliumlike transitions, their effects do result in a lack of better agreement with what is published in Ref. [3].

The predicted population in both the $2p3d$ $^3F_3$ and $^3F_4$ levels is large relative to the populations of other nearby energy levels because there are no electric dipole decays to any of the ten lowest lying energy levels (those coming from the $2s^2$, $2s2p$, and $2p^2$ configurations). The calculations done using RELAC reveal that there are $M2$ decays from the $2p3d$ ^3F states to the $2p^2$ ^3P states, and $E2$ decays from the $2p3d$ ^3F states to the $2s2p$ ^3P states. However, when compared to the $E1$ decay rates between $2p3d$ ^3F and $2p3p$ ^3D, the $M1$ and $E2$ decay rates are several orders of magnitude smaller. For the kinetics of the $2p3p$ $^3D - 2p3d$ ^3F considered here, the above CR equation is adequate. A discussion of the equilibrium conditions for O V and the effects of plasma conditions on the brightness of O V emission in the TEXT tokamak can be found in Ref. [4].

Oxygen is generally present in tokamak experiments at about the 1.5% level. At this concentration, transitions between $2p3d$ $^3F - 2p3p$ ^3D are predicted to be bright enough to be measurable in a typical tokamak plasma. Indeed, the lines predicted by RELAC at 6534 and 6567 Å are found to be present in typical survey spectra taken on the DIII-D tokamak with the seven chord multichannel divertor spectrometer (MDS) [11] at wavelengths approximately 70 Å shorter than the predictions, consistent with the previous observations of Bockasten and Johansson [5]. Table I lists the computed wavelengths and brightnesses for two bright visible transitions which are observable under reasonable experimental conditions, along with the spectroscopically determined precise wavelengths. The CR brightness for each transition in the model was calculated at an electron temperature of 50 eV and an electron density of 10^{13} cm^{-3}.

Identification of the two lines in the tokamak spectra is confirmed in three ways: (1) localization of the radiation to the expected region of the plasma, (2) near constancy of the intensity ratio between the two lines, and (3) by comparison of the temporal behavior during the discharge with known O V radiation measured simultaneously by a UV spectrograph. Figure 2 shows schematically the viewing geometry of the seven MDS chords. The O V distribution in the plasma is determined by a combination of the local source function at the surfaces, the parallel flow and cross-field transport of the ions, and the ionization and recombination rates. Because of finite diffusion and the thermal nature of the background electron distribution, the O V ($V_{pot} = 114$ eV) will exist in a temperature range of $40 < T_e < 140$ eV, and the radial

FIG. 1. Levels of the $2p3l$ ($l=s,p,d$) configurations grouped by LS multiplet. The number above each multiplet is the sum of the CR steady state population in each level of the multiplet.

TABLE I. Results of collisional-radiative models and current observations.

Transition	Predicted wavelength (Å)	Predicted brightness (rel)	Reported wavelength[a] (Å)	Observed wavelength (Å)	Observed brightness (rel)
$2p3p\ ^3D_3-2p3d\ ^3F_4$	6567	100.0	6500.24	6500	100.0
$2p3p\ ^3D_2-2p3d\ ^3F_3$	6534	41.4	6466.13	6465	50.0

[a]See Bockasten and Johansson, Ref. [5].
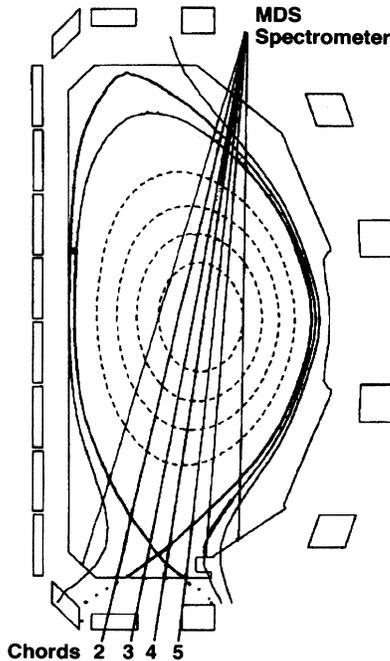
FIG. 2. Cross section of DIII-D tokamak, showing the seven MDS spectrometer channel views, with channels 2, 3, 4, and 5 indicated by straight lines extending from the MDS downwards toward the floor.
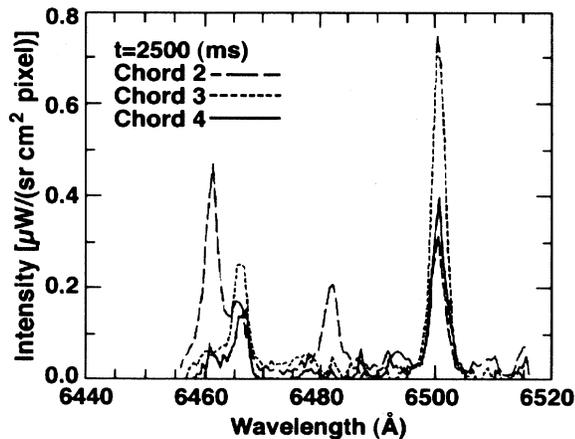
profile will be roughly Gaussian in the midplane of a poloidally diverted tokamak, centered at about $T_e = 70$ eV. Figure 3 shows the spectra for three of the seven spatial chords in the 6420–6550 Å range during a Ohmic portion of a tokamak discharge whose magnetic equilibrium can be described by the contour lines of flux indicated in Fig. 2. The two O v lines are found to be prominent only in the two channels which pass through either side of the divertor x point (channels 2 and 3) and they are weaker in channel 4. Their signals are down in the noise in the spectra of the other four channels of the MDS. These observations are easily interpreted to mean that the emission at the two wavelengths predicted for O v is spatially localized to the region around the separatrix, as is expected.

The identification of the two lines as O v is further confirmed by the comparison of the time behavior of the two lines relative to that of known O v lines measured simultaneously with a dual SPRED EUV spectrometer (extreme ultraviolet region, below 900 Å), which views the plasma tangentially through the center of the plasma in the midplane. Figure 4 shows the similarity in time behavior of the visible and UV O v lines. Further confirmation of the measured lines as O v comes from the examination of other tokamaks's spectra. So far, the two prominent O v lines in the visible at the same wavelengths have been found in survey spectra of the TEXT tokamak [12].

The brightness prediction and rediscovery of the pair

FIG. 3. Spectra from channels 2 (long dash), 3 (short dash), and 4 (solid) in the 6450–6520 Å range at 2500 ms during shot 75 591 on the DIII-D tokamak. The two visible O v lines are present on all three channels. Two bright C III lines are present only on channel 2 which views the inner strike point (refer to Fig. 2).
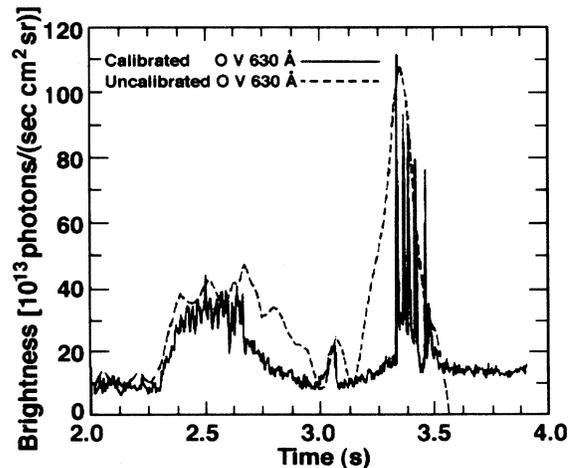
FIG. 4. Time evolution during the shot 75 591 of the normalized O v line brightness at 6500 Å, vs the multiplet near 630 Å measured simultaneously by the calibrated SPRED EUV spectrograph.

of visible O V lines in a plasma demonstrate the value of cross-disciplinary study: the HULLAC codes, which are used to make predictions for higher-Z ions in non-tokamak plasmas by the atomic physics community, is found to explain common features of a visible tokamak spectrum of interest to the fusion community. Further, the gap is bridged between visible and UV spectroscopy on tokamaks, which are usually done by different practitioners. As this work stands, a practical way of determining the distribution and concentration of O V in a tokamak has been identified. This work can be readily extended in a number of directions: Predictions for other ions can be made in an effort to identify other interesting atomic systems useful as passive observables in fusion studies. These same spectral lines may also be present in other plasmas such as the solar corona. The use of the diagnostic line brightness technique for remote passive measurement of T_e and n_e could perhaps be extended to the more readily measurable visible region.

The immediate precedent of the present work was a set of 98-level calculations for the Ne VII ion, made in preparation for an experiment on the TORE SUPRA tokamak, in which changes in the boundary layer T_e and n_e induced by an ergodic divertor perturbation were to be measured using established line brightness ratio techniques on injected trace levels of neon [13]. Such techniques had been successfully used using O V on the TEXT tokamak during ergodic magnetic limiter experiments [14].

In addition to passive measurement, the highly populated upper levels of ions such as O V can make suitable targets for laser-fluorescence diagnostic schemes [15]. This technique has the advantage that by crossing the measurement with the excitation laser, the measurement is local, and yields both T_i from the line shape, and n_i from the intensity of the line. A database of higher-level transitions would probably lead to the discovery of other useful excitation schemes.

In conclusion, using the HULLAC package, a 98-energy-level, collisional-radiative atomic model of Be I–like oxygen was generated, and wavelengths and brightnesses of transitions within the $n = 3$ level of O V have been calculated for tokamak-relevant conditions of T_e and n_e. The two brightest transitions in the visible within this ion have been easily measured on the DIII-D tokamak. The confirmation of these lines has been made by the constancy of the ratio between them, their spatial location, the similarity in their behavior to known O V lines in the ultraviolet, and agreement in wavelength with previous spectroscopic measurement. A cursory examination of the spectra from other tokamaks suggest that these lines are common. Combined with information about the background plasma, these lines can provide a rough measure of oxygen contamination and a constraint on impurity transport simulations in tokamak. The possible extension of the line brightness ratio technique for diagnosis of fusion or remote plasmas using visible radiation from ionic systems such as O V should be further explored. Other diagnostic uses, such as in the laser fluorescence technique, also profitably employ the data that HULLAC can generate, and are motivating further investigation of this type of atomic system.

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