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EFFECTIVE K α X-RAY EXCITATION RATES
FOR PLASMA IMPURITY MEASUREMENTS

By

K.W. Hill et al.

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EFFECTIVE $K\alpha$ X-RAY EXCITATION RATES FOR PLASMA IMPURITY MEASUREMENTS

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ABSTRACT

Metal impurity concentrations are measured by the Pulse-Height-Analyzer (PHA) diagnostic from $K\alpha$ x-ray peak intensities by use of an averaged excitation rate $\langle\sigma v\rangle$. Low-Z impurity concentrations are inferred from the continuum enhancement (relative to a pure plasma) minus the enhancement due to metals. Since the PHA does not resolve lines from different charge states, $\langle\sigma v\rangle$ is a weighted sum of rates; coronal equilibrium is usually assumed. The $\langle\sigma v\rangle$ used earlier omitted the intercombination and forbidden lines from the dominant heliumlike state. The result was an overestimate of metals and an underestimate of low-Z impurities in cases where metals were significant. Improved values of $\langle\sigma v\rangle$ using recent calculations for H-, He-, and Li-like Fe range from 10 to 50% larger than the earlier rates and yield metal concentrations in better agreement with those from VUV spectroscopy.

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1. INTRODUCTION

The importance of understanding impurity behavior in tokamak plasmas is evidenced by the numerous experiments and efforts devoted primarily or partially to impurity studies.¹⁻³ The absolute concentration of impurities can be measured readily from the soft x-ray Pulse-Height-Analysis (PHA) spectrum in the 1.5-20 keV range.³⁻⁵ Medium-Z (14-28) impurity concentrations are measured from K α line intensities by use of theoretical excitation rates. Since the PHA does not resolve lines from individual charge states, a sum of excitation rates for the various charge states weighted by their fractional abundance must be used.^{4,5} Low-Z concentrations are inferred from their contribution to the continuum due to bremsstrahlung and radiative recombination (measured by the continuum enhancement factor ζ). The latter determination requires a knowledge of which low-Z impurities are present, which is usually determined from VUV spectroscopy. The resistivity or effective Z, Z_{eff} , ensues from contributions due to the plasma and various impurity species.

For some plasma regimes in TFTR medium-Z impurity concentrations (Ti, Fe, Cr, Ni) have been relatively high (e.g., low density plasmas, plasmas constrained by a titanium-carbide-coated or Inconel limiter) and have constituted a significant fraction of the continuum enhancement factor. For these cases it is especially important to know the medium-Z impurity concentrations accurately, because their uncertainty can propagate to larger uncertainties in the low-Z impurity concentration. In fact, measurements both on the TFTR and PLT⁴ (Princeton Large Torus) tokamaks in certain plasmas with very high metal concentrations have indicated that the metal excitation rates used until now are somewhat too small.

Usually medium-Z impurities in the center of TFTR are predominantly in

the heliumlike state and are approximately in coronal equilibrium.⁶ However, in the so-called "energetic ion" regime,⁷ characterized by low electron density [$n_e(0) \sim 10^{13} \text{cm}^{-3}$] and high neutral-beam-heating power ($P_b \sim 5 - 10$ MW), both high metal concentrations and evidence of marked departures from coronal equilibrium are observed.⁸ The distribution shifts to lower charge states due to charge exchange of the metals with enhanced plasma neutrals. In these cases a knowledge of the excitation rates for individual charge states is important, so that the appropriate weighed average of excitation rates may be calculated.

In recent years, comparison of theoretical 1s-2p excitation rates with high resolution x-ray spectra of medium-Z elements from laboratory and astrophysical plasmas has led to refinements in excitation rates and identification and inclusion of important processes which were previously omitted or inadequately treated.^{6,9} These include excitation via dielectronic recombination, collisional resonances, cascading, and charge exchange with neutral plasma atoms. In this paper we have collected some of the latest theoretical excitation rates for iron, which include or improve upon some of the aforementioned effects.⁹ The resulting effective excitation rates for these metals range from 10 to 50% higher than rates used earlier in the electron temperature range 1.5-4.0 keV, typical in the center of TFTR, and result in lower inferred metal concentrations in the plasma. These findings help to resolve some earlier inconsistencies in which the continuum enhancement factor for the metals could be, in extreme cases, larger than the total enhancement factor, leaving no room for carbon and oxygen. In Sec. II we briefly describe the technique of metal impurity measurement with the PHA. In Sec. III we discuss the excitation rates, and in Sec. IV we describe the differences between the new rates and those used previously.

II. METHOD OF IMPURITY ANALYSIS

The concentration of a medium-Z impurity m is inferred from the $K\alpha$ x-ray peak intensity I by the equation

$$I = n_e n_m S_{\text{eff}}(T_e), \quad (1)$$

where n_e is the electron density and S_{eff} is an electron-temperature-dependent effective excitation rate. Since the PHA diagnostic does not resolve individual x-ray lines ($E = 220$ eV FWHM), S_{eff} is a double sum, first over the various lines j emitted by a given charge state, and then over charge states i , weighted according to their fractional abundance f_i ,

$$S_{\text{eff}}(T_e) = \sum_{i,j} f_i S_{ij}(T_e) \quad (2)$$

Once the concentrations of the medium-Z impurities are known, their contribution to the x-ray continuum enhancement factor and to the total ionic charge of the plasma can be calculated. The remaining enhancement is attributed to the fully stripped low-Z impurities,

$$\sum_{\text{Low-Z}} \zeta_i = \zeta - \sum_{\text{Med-Z}} \zeta_i - \zeta_p \quad (3)$$

where ζ is the total measured enhancement, and ζ_p is that due to the plasma species. The first sum is over low-Z impurities and the second sum over medium-Z species. Invoking charge neutrality of the plasma,

$$\sum_{\text{Low-Z}} n_i Z_i + \sum_{\text{Med-Z}} n_i Z_i + n_p = n_e \quad (4)$$

and using UV spectroscopy to identify the low-Z species, one can calculate the low-Z concentrations. In Eq. (4) the Z_i are the charges of the ions. If the medium-Z concentrations are high and are, in fact, overestimated due to use of excitation rates which are too small, the sum of low-Z enhancement factors in Eq. (3), and thus, the inferred low-Z concentrations, can be zero or negative. The occasional occurrence of this situation has prompted the present reassessment of excitation rates.

III. $K\alpha$ EXCITATION RATE CALCULATIONS

Since the purpose of this paper is to point out some recent improvements in $K\alpha$ excitation rates relevant to fusion plasma impurity measurements and to put them in a form suitable for use by diagnosticians, it is appropriate to review briefly the history of these rates. Following the early high resolution measurements of iron $K\alpha$ spectra on the ST tokamak,¹⁰ Merts *et al.*¹¹ made detailed calculations of rates for excitation of iron ions from Fe XIX to Fe XXV by both impact excitation and dielectronic recombination. It was subsequently shown by high resolution spectroscopy of Fe on PLT¹² that these calculations agreed reasonably well with measurements if a coronal equilibrium distribution of charge states was assumed: ionization rates of Lotz were used for $0.8 \text{ keV } T_e < 1.2 \text{ keV}$, but better agreement for $T_e = 1.5 \text{ keV}$ was obtained if Griem's suggestion of using $0.5 \times$ Lotz ionization rates was followed. Thus, it was concluded that a reasonable effective excitation rate for PHA measurements could be obtained by summing the individual charge-state rates weighted according to coronal equilibrium.⁴

Later Bitter made very high resolution measurements on PLT of Fe XXV and the neighboring dielectronic satellite spectra,¹³ and compared them with the detailed calculations of Bely-Dubau.¹⁴ The dielectronic recombination rate

coefficient inferred from the PLT data agreed well with theory. Subsequent comparisons of the Ti XXI spectra and satellites from TFTR with calculations of Dubau showed excellent agreement.⁶ Thus, since the heliumlike charge state is the dominant contributor to the K α radiation from titanium and iron, replacing the less detailed rates of Cowan by these newer calculations should significantly improve the validity of the resultant effective excitation rate.

In this paper total effective excitation rates from iron were calculated as a sum of rates for charge states Fe XIX - Fe XXVI, weighted according to coronal equilibrium calculations by Breton.¹⁵ The individual charge-state rates were approximated by best fit parametric expressions which were accurate in most cases to 1 - 2% over the temperature range of interest. Also the charge state abundances were parameterized by eight-term polynomials which were generally valid to better than 2%. Thus the accumulation of error in the total rates may be -5 - 8% at worst for $T_e > 1.5$ keV, since practically only Fe XXIV and Fe XXV contribute. The errors over most of the range of interest are probably smaller.

IV. DISCUSSION

The weighted rates for individual charge states as well as the total rate summed over all charge states are shown in Fig. 1. Weighted rates were graphed because they indicate which charge states are important in each temperature range. We can see that Fe XXV, with small contributions from Fe XXIV, is practically the only contributor for typical central TFTR temperature of 1.5 - 4 keV. For Fe XIX - Fe XXIII rates from Cowan were used. These along with Cowan's values for Fe XXIV and Fe XXV have previously been presented by von Goeler.⁴ The new information in Fig. 1 is the curves for Fe XXIV - Fe XXVI, which were taken from Bely-Dubau⁹ and include some effects not treated

by Cowan. In fact, the Fe XXVI curve consists of contributions to lines w, x, y, and z (upper levels $1P_1$, $3P_2$, $3P_1$, $3S_1$, respectively) due to radiative and dielectronic recombination of Fe XXVI, which were not treated by Cowan at all. This contribution is significant only for $T_e > 5$ keV. The impact excitation contribution to Fe XXVI was not included because it is well separated in energy from the Fe XIX - Fe XXV peaks and can readily be resolved by the PHA. To complete the information, Cowan's rates for excitation by dielectronic recombination of Fe XXIV to Fe XXIII, which were not calculated by Dubau, were added to Dubau's impact excitation rates for Fe XXIV.

The effect of using the larger rates for Fe XXIV and Fe XXV, as well as including contributions from Fe XXVI, can be seen from Fig. 2. These curves are either the ratio of rates of Dubau to those of Cowan (Fe XXIV and Fe XXV), or the ratio of the total effective rate using the mixture of Cowan's and Dubau's rate described earlier to the effective rate using only contributions calculated by Cowan. The curves marked "Lotz" and "Griem" indicate that the ionization equilibrium was calculated differently only for Cowan's total rates. For the "Lotz" curve ionization rates of Lotz were used in the equilibrium calculations, whereas one-half the ionization rates of Lotz (as suggested by Griem) were used for the "Griem" curve. The total curves in Fig. 2 indicate that, for typical central TFTR temperatures (1.5 - 4 keV), the present effective excitation rate is larger than the earlier effective rates from Cowan by 10-50% for "Lotz" equilibrium and 30-50% for "Griem" equilibrium. The net effect is a proportional reduction in the measurement of iron concentration in TFTR.

Figure 2 shows that Dubau's excitation rate for Fe XXIV is generally larger than that of Cowan, and the ratio increases with temperature. This is due to the fact that Cowan uses a Van Regemorter type formulation for impact

excitation with a constant oscillator strength, whereas Dubau uses distorted wave methods similar to Vainshtein.¹⁶ Vainshtein¹⁷ has done elaborate calculations and shown that exchange effects can significantly alter the excitation rate coefficients. As in Fig. 1 both numerator and denominator in Fig. 2 for the Fe XXIV curve include an impact excitation contribution and a dielectronic excitation contribution. Since Bely-Dubau presented only impact excitation in her report,⁹ Cowan's dielectronic excitation was used both in the numerator and denominator. Dubau uses a distorted wave approximation for the scattering problem and finds that his collision strengths agree well with those of Sampson.¹⁸ Contributions from excitation to states with $n > 2$ followed by cascading are not included since they are expected to be small due to the predominance of autoionization over radiation for these states.

The main reason for the ratio (Fe XXV) in Fig. 2 of the Dubau to the Cowan excitation rate of Fe XXV being greater than one is Dubau's inclusion of lines x, y, and z, which Cowan did not calculate. Furthermore, Dubau included the effect of excitation to levels with $n > 2$ followed by cascading. For an electron temperature of 2.6 keV this increased lines w and y slightly, decreased line x slightly, and increased line z by a factor of 3, resulting in a net increase of 17% for all 4 lines. Dubau also showed that the effect of collisional resonances on the excitation processes is negligible for Fe XXV.

V. CONCLUSIONS

Since previous analysis of TFTR PHA data was done using Cowan's rates with "Griem" equilibrium, Fig. 2 shows that use of the present rates will reduce the concentration of iron (also Ti, Cr, and Ni) by 30-50%. Thus the low-Z concentrations and Z_{eff} will be increased somewhat at low densities, where metals make a noticeable contribution to the continuum enhancement. The

new increased rates are more consistent with measurements made in extreme cases of plasmas with very high metal concentrations ($n_m \sim 5 \times 10^{-3} n_e$), where domination of the enhancement factor ζ [Eq. (3)] by medium-Z impurities could practically put a lower limit on the effective medium-Z excitation rate.

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FIGURE CAPTIONS

Fig. 1. Total effective K α x-ray excitation rate for iron calculated as a sum of rates for charge states Fe XIX - Fe XXVI (Fe XXVI is 25 times ionized iron) weighted according to a coronal equilibrium distribution from Ref. 14. Also shown are the (weighted) contributions from the individual charge states. Data for Fe XXV and Fe XXVI and the collisional impact excitation contribution for Fe XXIV were taken from Ref. 8. The remaining contributions were taken from data presented in Ref. 4.

Fig. 2. Ratio of iron rates from Ref. 8 to those from Fig. 10 of Ref. 4 for Fe XXIV and Fe XXV. Also shown are the ratios of the "Total" curve from Fig. 1 to the curves marked "Lotz" and "Griem" in Fig. 10 of Ref. 4.

Fig. 1

Fig. 2

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