ANALYSIS OF QUASI-CONTINUUM BANDS AND LINE SPECTRA OF HIGHLY IONIZED W and Au

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Résumé

Dans la présente étude, on montre que l'étroite bande de rayonnement quasi-continu émise entre 40 et 100 Å par le plasma d'éléments lourds (Z>50) dans des conditions fort différentes (plasma créé par laser, étincelle sous vide, ou Tokamak) provient du mélange d'un grand nombre de raies correspondant aux transitions $\Delta n=0$, n=4. Les calculs des faisceaux de transitions non résolues (UTA) montrent, en effet, que pour près de vingt degrés d'ionisation consécutifs, les transitions de résonance sont émises dans un domaine très étroit de longueurs d'onde. Les calculs, présentés ici pour le cas de l'or et du tungstène ont été effectués à l'aide de nouvelles formules UTA qui incluent les effets de mélange de configurations. Cette étude permet l'extension des résultats obtenus précédemment pour les terres rares.

Abstract

The spectra of heavy elements (Z > 50) observed in laser-produced plasmas, vacuum sparks and Tokamaks are characterized by a strong quasi-continuum band emitted in the 40-100Å range. This band originates from the blending of a great number of lines emitted in the $\Delta n=0$, n=4 transitions. Indeed, the Unresolved Transition Array (UTA) computations show that for about twenty adjacent ionization states, the mean wavelength of the main resonance transitions remains in a very small wavelength range. The results of these computations are given here for tungsten and gold. The computations rely on new UTA formulae which include the effect of configuration mixing. This work extends the previous results obtained for the rare-earths spectra.

I. Introduction

Spectra of heavy elements (Z > 50) observed in laser-produced plasmas [1] and vacuum spark [2] or emitted by intrinsic [3,4] or injected [5,6] impurities in Tokamak plasmas are characterized in particular by a strong quasi-continuum band in the 40-100Å range. This band originates from the blending of hundreds or thousands of spectral lines corresponding to 4-4 transitions between complex configurations in many ionization stages of the element involved. In order to interpret these bands, one has to compute the wavelength of the resonance transitions (or the mean wavelength in the case of complex arrays) in the different ionization stages involved. So far, due to the complexity of the calculations, this has been done only for W XXXIII to W XXXVII [3] and for W XXVIII [7], and for the relatively simple RhI- (ground state $4d^9$), RuI- ($4d^8$), SrI- ($4d^2$) and RbI-like ($4d^1$) isoelectronic sequences in the rare-earths [2].

II. Theory

Mean wavelength of complex transition arrays can be computed in a relatively simple manner using the UTA (Unresolved Transition Array) model [8]. This model gives the average and the variance of the line-strength weighted distribution of transition energies from which one can infer the mean wavelength and width of the spectral distribution of the lines (see ref. 2). Moreover, a method for handling configuration mixing in the framework of the UTA model has been recently developed [9]. This mixing is particularly important for the $4p^64d^n$-$[4p^54d^{n+1}+4p^64d^{n-1}4f]$ transitions [2]. In the rare earths case, it has been shown [2] that this mixing causes a quenching of the long wavelength transitions, leading to a narrowing of the spectral width of the band for each ion, and moreover to a superposition of these bands for many ionization stages, from n = 1 to 9, in agreement with the observed narrow bands.

III. Tungsten spectra

Computations of resonance transitions have been performed for W XXIV to W XXXXIV, using the UTA method for the complex transitions, and individual energy level ab-initio computations based on RELAC code [10] for the simpler sequences.

The ground state of W XXIV to W XXVIII is $4d^{10}4f^n$ (n = 5 to 1) and the resonance transition is $4d^{10}4f^n$-$4d^94f^{n+1}$. In this kind of transitions, the isolated configuration approximation is valid [11]. Thus,the simple UTA formula was used. In the AgI-like sequence (n=1), the results compare well with the published computations [7].

For W XXX to XXXVIII, the ground configuration is $4p^64d^n$ (n=9 to 1). The resonance transition is $4p^64d^n$-$[4p^64d^{n-1}4f+4p^54d^{n+1}]$. As pointed out by Cowan [12], the $4p^64d^n$-$4p^54d^{n+1}$ transition is split due to the 4p spin orbit integral, and the $4d^n$-$4d^{n-1}4f$ transition falls between the two subarrays. This situation is thus somewhat different from that encountered in the same isoelectronic sequences for the rare-earths. Nevertheless, mixing of the arrays is strong and also causes the quenching of the long wavelength side of the arrays. This is shown in Fig. I where ab-initio computations of the $4p^64d^n$-$[4p^54d^{n+1}+4p^64d^{n-1}4f]$ transition are given as synthetic plots for RuI-like (n=8) and SrI-like (n=2) tungsten. These plots show that the mean wavelength of the bulk of the transition intensity remains between 45 and 50Å, even though some weaker lines appear for the SrI-like spectrum at longer wavelength. Computations performed for all the ionization states, n = 9 to n = 1, using UTA model and quenching formulae show the same results. This strong effect of configuration mixing should be included in the intensity model for diagnostic application proposed by Cowan [12] based on the intensity ratio between the central 4d-4f array and the two 4d-4p adjacent subarrays.

For W XXXIX to W XXXXIV, the ground state is $4s^24p^n$ (n=6 to 1). The resonance transition is $4s^24p^n$-$[4s4p^{n+1}+4s^24p^{n-1}4d]$. Mixing between the two upper configurations is expected to be strong. But since the transitions are simpler, full calculations in intermediate coupling using the RELAC code were performed.

Examples of results are given in table I. For W XXIV and W XXXIV the mean wavelength of the transition computed with the UTA model is given. In the two other cases the most intense line of the transition is given.

These results, representative of all the computations for W XXIV to W XXXXIV, show that for all the ionization stages involved, the strong lines fall in a small range between 46 and 5IÅ. Table I gives also the results for Au showing the same trend.

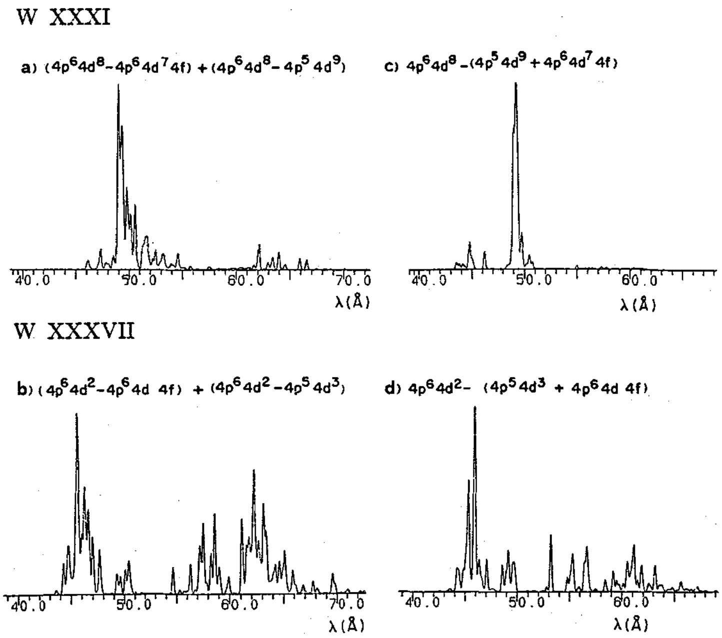

Figure I

Synthetic spectra of the computed arrays for W XXXI (a,c) and W XXXVII (b,d); a,b - superposed arrays, c,d - mixed arrays

TABLE I

Transition	Ion	λ(Å)	Ion	λ(Å)
$4d^{10}4f^5-4d^94f^6$	W XXIV	50.114	Au XXIX	43.618
$4p^64d^5-[4p^54d^6+4p^64d^44f]$	W XXXIV	50.565	Au XXXIX	43.956
$4p^6-4p^5_{1/2}4d_{3/2}$	W XXXIX	46.061	Au XXXXIV	37.839
$4p_{1/2}-4d_{3/2}$	W XXXXIV	47.417	Au XXXXIX	38.601

IV. Conclusions

The remarkable wavelength constancy of the strong emission band emitted by tungsten plasma in the 48-53Å range as observed from various sources [3, 4, 13], under different conditions, is explained by the present calculations, which show that, for about twenty ionization states, the mean wavelength of the resonance transition remains in a very small wavelength range. This is in part due to the strong configuration mixing in configurations involving 4d open shell [2,9] which causes no appreciable change of the mean wavelength from 4d-4f transitions (in $4d^n$ or $4f^n$ ground configuration ions) to 4p-4d transitions (in $4p^n$ ground configuration ions).

References:
1. O'Sullivan, G., and Caroll, P.K., J. Opt. Soc. Am., 71, 227 (1981).
2. Mandelbaum, P., Finkenthal, M., Schwob, J.L., Klapisch, M., Phys. Rev. A35, 35, 5051 (1987).
3. Isler, R.C., Neidigh, R.V., and Cowan, R.D., Phys. Lett. 63A, 295 (1977).
4. Hinnov, E., and Mattioli, M., Phys. Lett. 66A, 109 (1978).
5. Finkenthal, M., Lippman, A.S., Huang, L.K., YU T.L., Stratton, B.C., Moos, H.W., Klapisch, M., Mandelbaum, P., Bar Shalom A., Hodge, W.L., Phillips, P.E., Price, T.R., Porter, J.C., Richards, B., and Rowan W.L., J. App. Phys. 59, 3644 (1986).
6. Hinnov., E., Beiersdorfer, P., Bell, R., Stevens, J., Suckewer, S., von Goeler, S., Wouters, A., Dietrich, D., Gerassimenko, M., and Silver, E., Phys. Rev. A35, 4876 (1987).
7. Sugar, J., and Kaufman, V., Phys. Rev. A21, 2096 (1980).
8. Bauche-Arnoult, C., Bauche, J., and Klapisch, M., Phys. Rev. A20, 2424 (1979).
9. Bauche, J., Bauche-Arnoult, C., Klapisch, M., Mandelbaum, P. and Schwob, J.L., J. Phys. B,20, 1443 (1987).
10. Klapisch, M., Schwob, J.L., Fraenkel, B.S. and Oreg J., J. Opt. Soc. Am. 67, 148 (1977).
11. Bauche, J., Bauche-Arnoult, C., Luc-Koenig, E., Wyart, J.F. and Klapisch, M., Phys. Rev. A28, 829 (1983).
12. Cowan, R.D., The Theory of Atomic Structure and Spectra, University of California, Berkeley, 1981,p. 630.
13. Dewhurst, R.J., Khan, M.A., and Pert, G.J., J. Phys. B,8, 2301 (1975).