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IONIZATION MODEL FOR NICKEL-LIKE GOLD

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Introduction

Among various scheme proposed for population inversion, the one called "collisionnal excitation pumping" has lead the design of the LLNL experiment[1]. Neon-like ions were used. For the same scheme S. MAXON, P. HAGELSTEIN et al[2] have suggested the use of nickel-like tin (Sn^{22+}) in a gas puff experiment and Eu^{35+} in a laser experiment[4]. Nickel-like gold ions have been studied in laser plasmas[3] and can be used for the same purpose. Study of them is also worthwhile for temperature and density diagnostic and for checking of simplified ionization models.

Before we build an extensive population model for gold ionized 49 to 52 times, we have studied with a more simple model the effect of accounting for cascades (or dielectronic recombination) and $\Delta n = 0$ transitions. These transitions allow some understanding of typical feature of experimental gold spectra.

Electronic structure of ions

We first recall briefly the electronic structure of Nickel-like (Au^{51+}), Cobalt-like (Au^{52+}) and Copper-like ions (Au^{50+}).

Nickel-like ground state is a closed shell $3p^6 3d^{10}$, of which either 3d or 3p electron can be easily excited. The optically forbidden 3d-4d transition has a rather high collisionnal excitation rate ; the $3d^9 4d$ metastable levels can also be populated through desexcitation from the $3d^9 4f$ and $3p^5 3d^{10} 4s$ levels. This leads to a possibility of population inversion with the $3d^9 4p$ levels which are rapidly depopulated by spontaneous emission.

Similar transitions are found in Au^{50+}, but with one "spectator" electron which yields transition arrays instead of isolated lines. But the excited levels are more closely coupled and less subject to non equilibrium population, due to the proximity of the ionization limit. In Au^{52+}, transitions arrays are the consequences of the one more hole in the 3d subshell.

Seven hundreds of optically allowed lines had been computed by D. PAIN and J. BAUCHE[3] distributed among five successive ionization stages. For this study, one of us (J.B.) with his own multi-configuration Dirac Fock (MCDF) program, has compute about thirty thousands transitions, both allowed and forbidden, distributed among four ionization stages (Au^{49+} to Au^{52+}), for the n=3 to n=4 electronic jump. The wavelengths of the Zn-like $3d_{5/2}$-$4f_{7/2}$ transitions has been corrected by a factor of 1.004 as all correlations has not been accounted for in the MCDF runs for these lines.

The synthetic spectra shown further use the MCDF values.

Accounting for low-rate transitions

To demonstrate the effect of new transitions, even with low rates, added to a given population model, we shall present the case of a very simple CR model. The reader will understand that the conclusion stays for a more extensive model.

In the "coronal equilibrium" approximation, an excited level (i) is populated through direct collisionnal excitation from the ground state (0). Its population is found by balancing excitation rate with spontaneous radiative decay : $N_i = N_o C_{oi}/(\Sigma A_{ij})$. The line intensity is then $I_{io} = N_i A_{io} h\nu = N_o C_{oi} h\nu A_{io}/(\Sigma A_{ij})$. Using the collision strength f_{oi}, it comes :

$$I_{io} = N_o \cdot n_e B T_e^{\frac{1}{2}} \bar{f}_{oi} BR_i \exp(-h\nu/kT_e)$$

where $B = 3.2 \times 10^{-6}$ $eV^{\frac{1}{2}}$ cm^3 W, and BR_i is the branching ratio ($BR_i = A_{io}/\Sigma A_{ij}$).

In "LTE" approximation one will found $I_{io} = N_o/\omega_o\ C\ (h\nu)^3\ gf \exp(-h\nu/kT_e)$ where $C = 4.32 \times 10^7$ $W.eV^{-3}$.

These two widely used models yield both line intensities proportionnal to the oscillator strength, at least for the brightest line where $\bar{g} \simeq$ constant. They cannot reproduced for example the experimental line ratios for the three components of the 3d - 4p transition of Nickel-like gold Au^{51+} (cf. Fig 1).

In a complete population model, the excited level (i) is also populated by $\Delta n = 0$ transitions, (which total rate will be noted Q_i), and by downward transitions (cascades, dielectronic recombination,...) which total rate will be noted P_i. Depopulating transitions are collisionnal desexcitation towards ground state (with rate C_{io}), $\Delta n = o$ transitions (with rate Q'_i) and excitation ionization that we shall neglect in this study.

The line intensity is then given by

$$I_{io} = N_o \frac{C_{oi} + P_i\ Q_i}{C_{io} + A_{io}/BR_i + Q_i}\ C\ f_{io}\ (h\nu)^3$$

Due to the large number of energy levels (106 in Au^{51+}) of the complex with an electron excited on the $n = 4$ shell, assuming a constant value for Q'_i and P_i is a reasonnable approximation. In order to demonstrate the effects of the added transitions, we shall also assume that P_i do not depend of the level (i).

We can now easily turn on and off these entrance and exit channels by changing the values of P and Q. (Q' is deduced from Q by the detailed balance principle).

One can understand that, due to the $\Delta n = 0$ transitions, (when $Q_i \neq 0$).

OPENING NEW ENTRANCE CHANNELS TOWARDS SHORT LIVED LEVELS ENHANCES EMISSION OF THE "METASTABLE" LEVELS.

This yields better prediction of the Au^{51+} 3d - 4p lines (Fig 1). But a more impressive result is found on the 3d - 4f array.

FIG 1 experimental spectrum of the 3d - 4p array of gold (a), compared to synthetic spectra with only the gf values (b), or with this CR model (c). Ionization stages included range from Au^{52+} to Au^{49+}, with reduced population of 0.05, 1., 0.04 and 0.008.

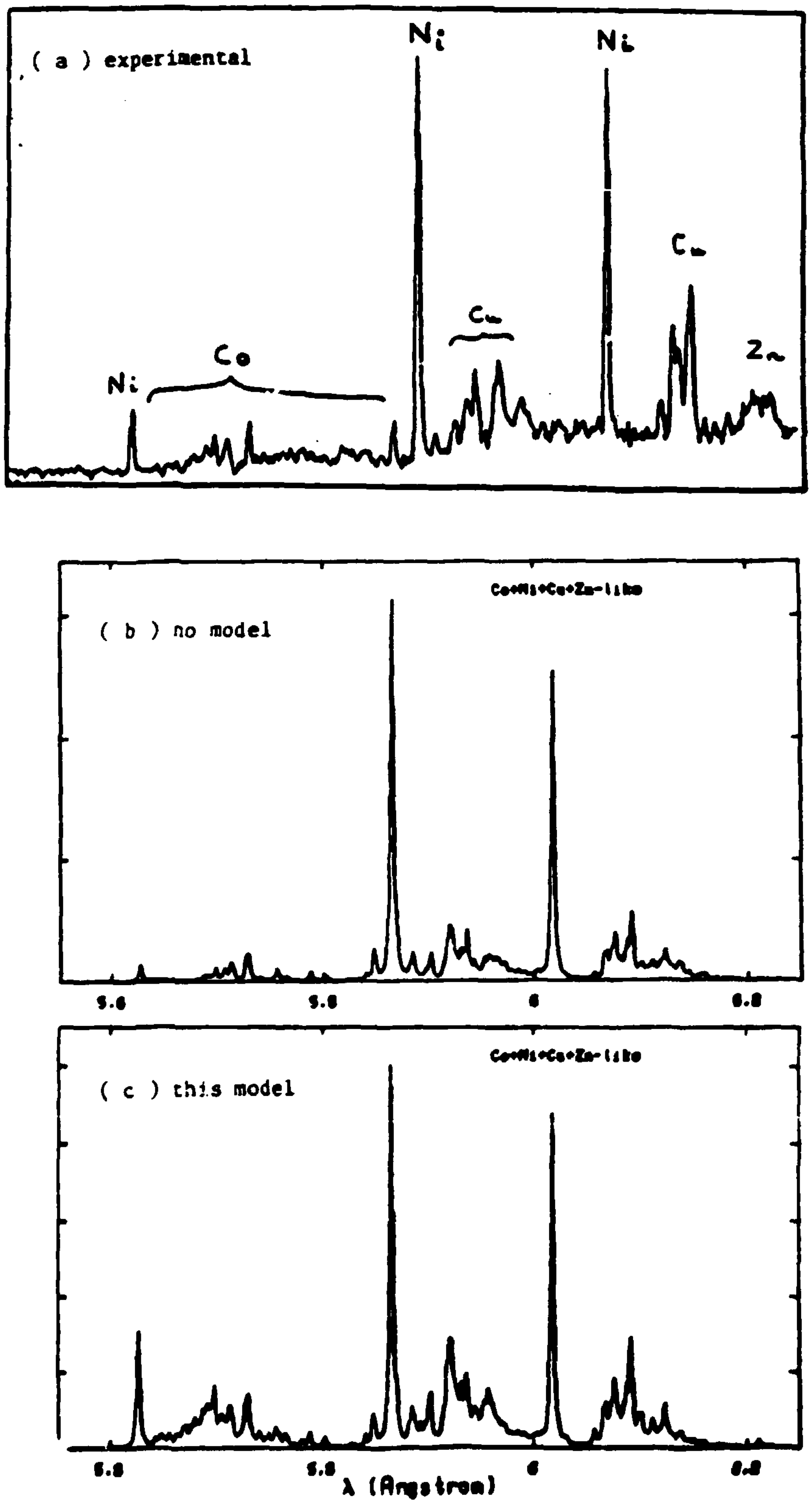
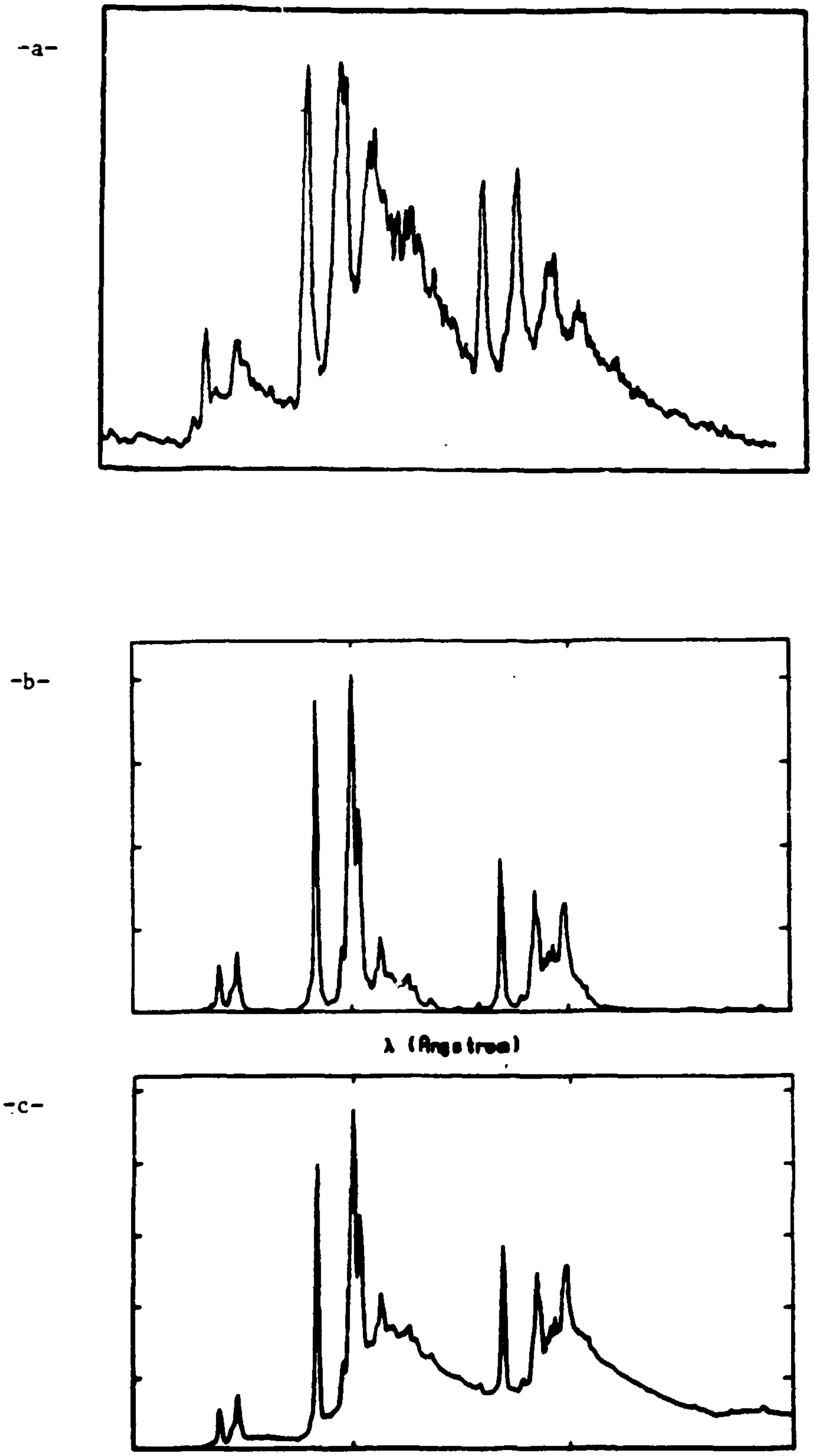


FIG 2 experimental spectrum of the 3d - 4f array of gold (a), compared to synthetic spectra with only the gf values (b), or with a red wing ($\Delta\lambda$ = 100 mÅ, P_{line}/P_{wing} = 0.3) added to each line (c).



It has been shown in a previous paper[3], that the experimental spectral shape of this array cannot be reproduced by convolution of a simple line profile with the line intensities deduced from their gf values. A phenomenological interpretation was that some satellite lines accompany each resonnance transition and give then a line profile with an extended (150 mÅ) red wing (Fig 2).

The piling up of these red wings reproduce the experimental understructure of the 3d - 4f array.

The simple CR model we have presented here, with the "coupling enhancement" of the low gf lines shows good construction of synthetic spectra (Fig 3).

However a reduced red wing (30 mÅ) still seems worthwhile, and means that other lines or mechanisms have to be added (Fig 4).

FIG 3 Synthetic spectra of the 3d - 4f array of gold obtained with this model. Populations are the same as in Fig 2. P = Q = 4.10^{11} s^{-1}

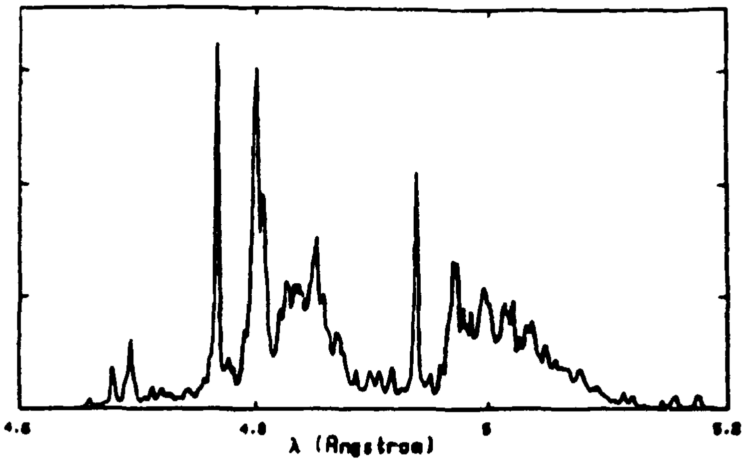
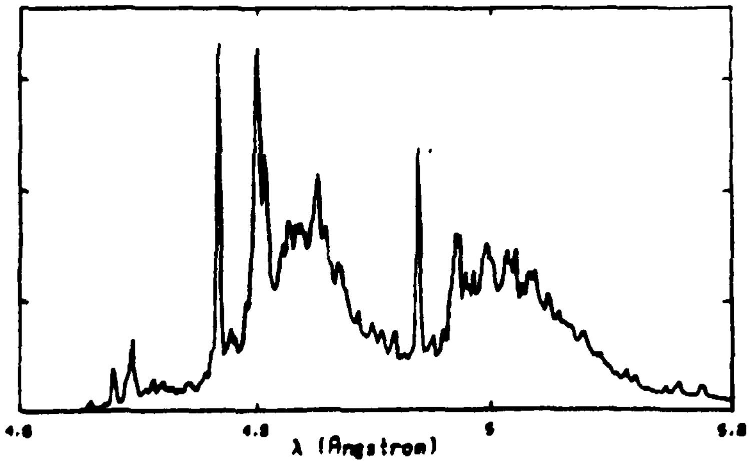


FIG 4 Same as Fig 3 but with a small (30 mÅ) red wing added.



Conclusion

The good agreement between experimental and synthetic spectra shows the importance of the cascades and $\Delta n = 0$ transitions. Recalling that in some case 90 % of the 3d - 4f array emitted intensity is found in the understructure, it becomes unaffordable to neglect these transition for power losses estimation, ionization/reconbination rates in ionization model and even detailed population model as it can dramatically change line intensity (or gain) ratios of different components of a same multiplet.

[1] PRL, 54(2), 106 and 110 (Jan. 85)
[2] JAP, 57(3), 971 (Feb. 85)
[3] Physica Scripta, 31, 137 (1985)
[4] JAP, 59(1), 293 (Jan. 85)