ATOMIC DATA for PLASMA MODELLING at LABORATOIRE AIMÉ COTTON,

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DETAILED INTERPRETATION of SPECTRA of ATOMS and IONS

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OPACITY and RADIATIVE POWER LOSSES

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GLOBAL METHODS for IONIC PROCESSES
MODEL of SUPERCONFIGURATION TEMPERATURES

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INTERPRETATION of COMPLEX SPECTRA of ATOMS and IONS

Experimental levels E_{exp} and wavelengths λ_{exp} compared with theory

λ_{calc} ,Landé factors g^{L}_{calc}, E1 transitions: $g^{upper}A$, $g^{lower} f$

theory = parametric (Racah-Slater) method by means of Cowan codes:

radial integrals and effective parameters for configuration interaction treated as adjustable parameters, eventually linked by Hartree-Fock (HFR) ratios

New experimental data, or critical surveys

Recent works (2007-2009)

Lanthanides: Nd^{3+}, Nd^{4+}, Tm^{3+}, Er^{1+}

complete determination and parametric description of $4f^{3}$ ground configuration in Nd IV

J. Phys B (2007) **40** 3957-3972; (2008) **41** 085001 (12pp)

Th. interp. and new energy levels in Er II, Wyart & Lawler, Phys. Scr. **79**, 045301 (2009)

In press : Ce^{3+}, Observation of Inner-Shell-Excited Configurations, Reader & Wyart (Phys. Rev A, accepted 08/2009)

In progress: Nd^{1+}, Tm^{1+}, Er^{3+}, neutral Er

tungsten:

Interpretation of the odd parity energy levels in the spectrum of neutral tungsten, J. Phys. B, Special Issue High Precision Atomic Physics, soon on-line

Recommended site for references on spectra

physics.nist.gov >>> Physical Reference Data > Bibliographic databases on Atomic Spectroscopy

not critically evaluated, but **frequently updated**

Short term future:

New observations of W spectra at Meudon (10.7m normal incidence spectrograph) in the range ~400-3000 Å, using phosphor image plates as detectors, in collaboration with ISAN (Troitsk, Russia) for the grazing incidence region. Unknown spectra of W^{7+} and W^{8+} .

Other works in LERMA, Meudon (W.-Ü L. Tchang-Brillet):

VUV Spectroscopy of HD and D2 molecules

A statement of support from the ADAS/ITER community to the high resolution Meudon facility able to produce data of fundamental interest might be crucially important for maintenance of the spectrometer

OPACITY AND RADIATIVE POWER LOSSES

fusion (tokamak and ICF), stellar physics

Complex spectra of mid-Z impurities (Au, …)
involving unresolved transition arrays or superconfigurations

Two approaches

Detailed level & line profile calculations

requires

a. Atomic database
(radiative transition energies, oscillator strengths)
provided by MCDF or Cowan's code

b. Precise lineshape
(electron, Doppler and ion Stark broadening)

Collaboration: Université de Provence (Marseille)

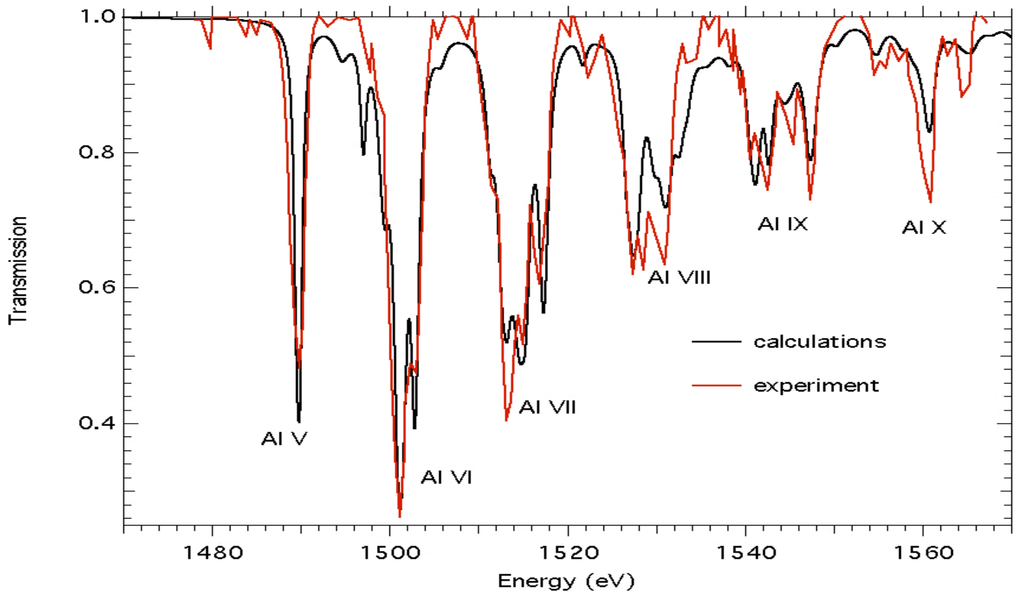
Detailed level & statistical distribution

requires

a. Atomic database
(radiative transition energies, oscillator strengths)
provided by MCDF or Cowan's code

b. Statistical distributions
(high-order moments)

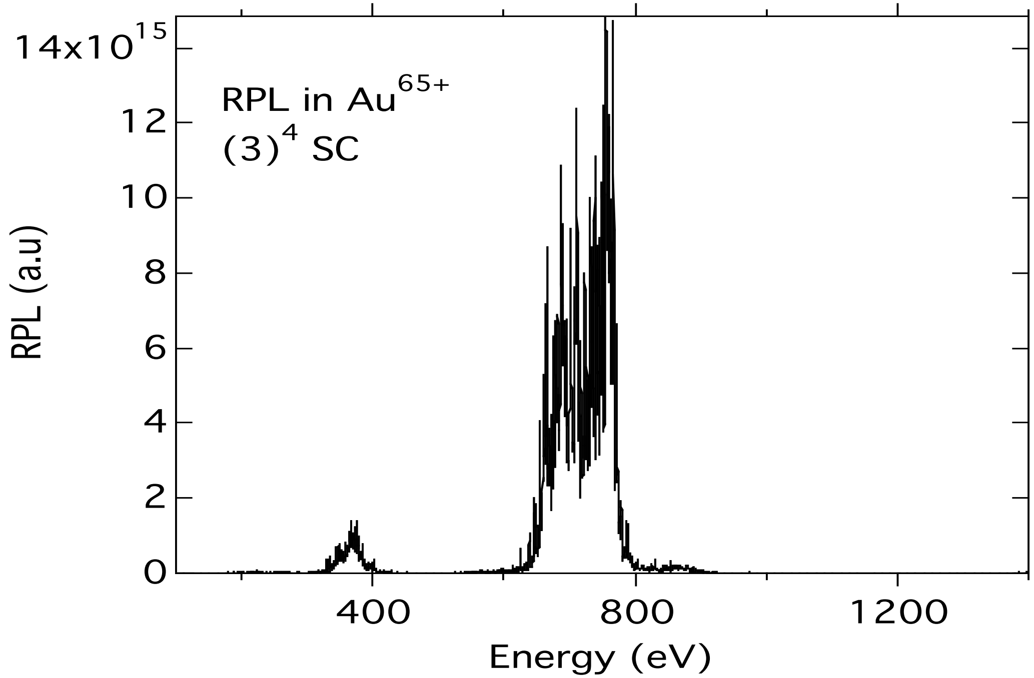
Collaboration: CEA



1s-2p transition array in Al plasma
(N_e=5×10^{22} cm^{-3}, kT_e=50 eV)

Experiment: P. Audebert et al
PRL **94**, 025004 (2005)

Calculations: D. Benredjem et al
HEDP **5**, 187 (2009)



N_e=10^{24} cm^{-3} T_e=12 keV
Apparatus FWHM=1 eV

important Doppler broadening
negligible ion Stark broadening

D. Benredjem et al
IFSA 2009 proceedings

GLOBAL CALCULATIONS FOR HOT PLASMA SIMULATIONS

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The need for global approaches

The dynamical equilibrium of the ions in hot plasmas is calculated through the use of the collisional-radiative (quantum) model (CRM), in order to account for the permanent change of the J-level of each ion, through a dozen of atomic processes. Because the number of atomic levels can reach millions, resorting to global methods is most desirable.

Instead of the standard CRM codes for levels, other ones run with level ensembles, i.e.,

- configurations, defined as sets of subshells $n\ell$ [1]
- superconfigurations, defined as sets of shells n [2]

For example, the configuration ensemble ($3s^2$, 3s3p, 3s3d, $3p^2$, 3p3d, $3d^2$) is the superconfiguration (SC) denoted $(3)^2$, i.e., all the configurations with 2 electrons in the shell n = 3.

Such a globalisation is made possible and efficient by the existence of effective temperatures within those ensembles. For example, the population of an SC in an ion reads

$$N(SC_i) = g(SC_i)\, n(ION)\, e^{\left(-\frac{E(SC_i)-E(SC_1)}{kT(ion)}\right)} \quad \text{(see Fig. 1)}$$

where g(SC) is the degeneracy of the SC and E(SC) the average value of the energies of the levels belonging to the SC.

An analogous formula can be written for the population of a configuration, depending on the effective temperature T(SC), defined within the SC [3].

In the Local-Thermodynamic-Equilibrium (LTE) limit, T(ion) and T(SC) are equal to T_e (the temperature of the free electron gas), otherwise T(ion) and T(SC) are determined through specific CRM calculations.

In the case of low density plasmas, good results are obtained when both configurations and SCs are introduced: a parameter q is defined and the SCs having less than q configurations are represented in the CRM by the configurations themselves [4]. In the example of a Gold plasma where Ne = 10^{12} cm^{-3} and Te = 2500 eV, the EBIT-II experiment leads to $\langle Z \rangle = 46.8 \pm 0.75$ whereas the calculations give 46. 4, after adjustement of the q value (see Fig. 4).

The plasma properties which can be modelled in that way

- the **charge-state distribution** (see Fig. 2)

- the **monochromatic emissivity**, i.e., the spontaneous-emission spectrum.

Due to the line broadening by numerous quantum and experimental effects, the lines usually coalesce into broad bands called Unresolved Transition Arrays (UTAs)[5]. Formulas have been derived for the first moments μ_n of the wavenumber distribution of the lines, weighted by their strengths. Then, each band can be represented by a Gaussian whose axis is given by μ_1, the variance by $\mu_2 - \mu_1^2$ etc. When the spin-orbit interaction is large, the arrays split into sub-arrays which are represented by separate Gaussians (see Fig. 3) [6].

- the **integrated emissivity**, i.e., the radiative power loss (RPL).

- the **opacity**, i.e., the radiative-absorption spectrum.

The Rosseland mean, which is a basic quantity for describing the transparency of the plasma, is extremely sensitive to the gaps -low-absorption wavenumber ranges- in the spectrum. The modelisation of the arrays by smooth Gaussians is no more suitable and a statistical method is used for introducing the levels in the Resolved Transition Arrays model (RTA) [7], without resorting to a level-by-level calculation (compare Figs. 5 and 6).

Plasmas of Germanium, Xenon, Tungsten, Gold, etc. have been modelled in that way for numerous values of the free-electron density and temperature. Many results have been presented at the NLTE Workshops organized by Yu. Ralchenko et al. Special attention has been given recently to Tungsten plasmas [8].

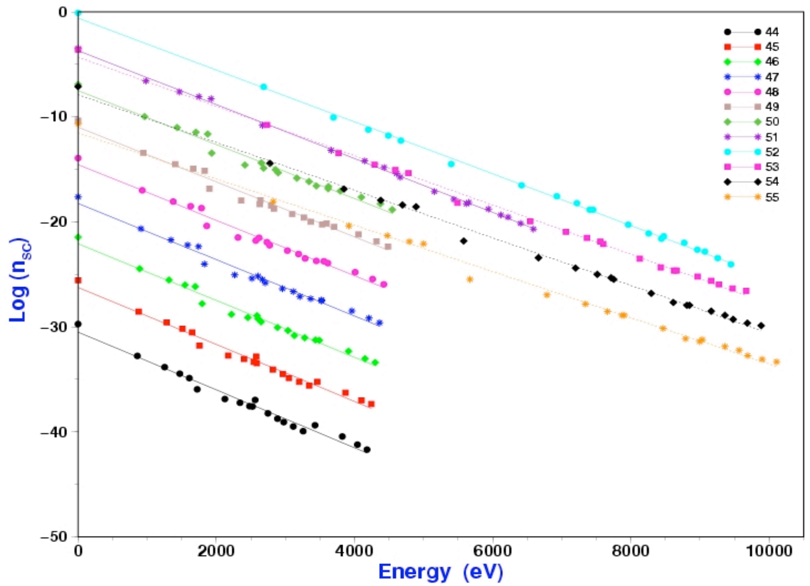

Fig. 1 T(ion) deduced from the slopes of the lines, for 12 ions in a Gold plasma (Te =2 500 eV, Ne=10^{22} cm^{-3})

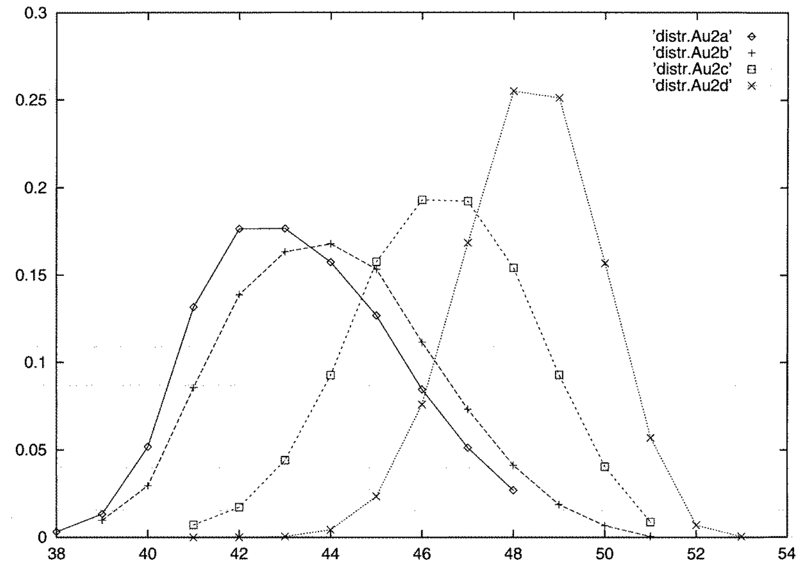

Fig. 2 Charge state distribution in Gold plasmas (Te = 1500 eV, Ne = $10^{19} \rightarrow 10^{22}$ cm^{-3})

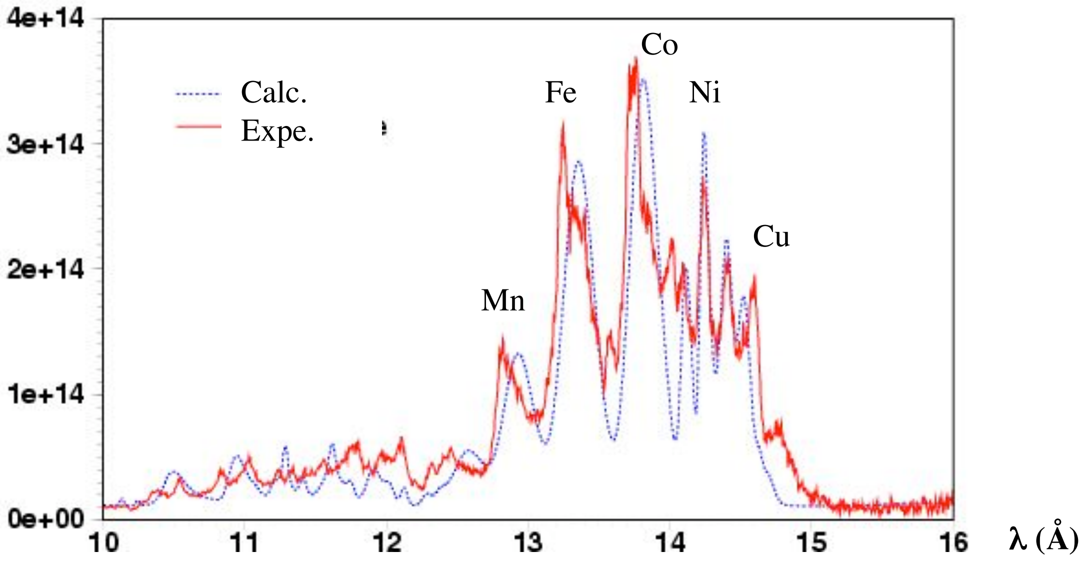

Fig. 3 Emission spectrum of Xenon. 3d - 4f transitions. Te = 450 eV, Ne = 1.2 10^{20} cm^{-3}

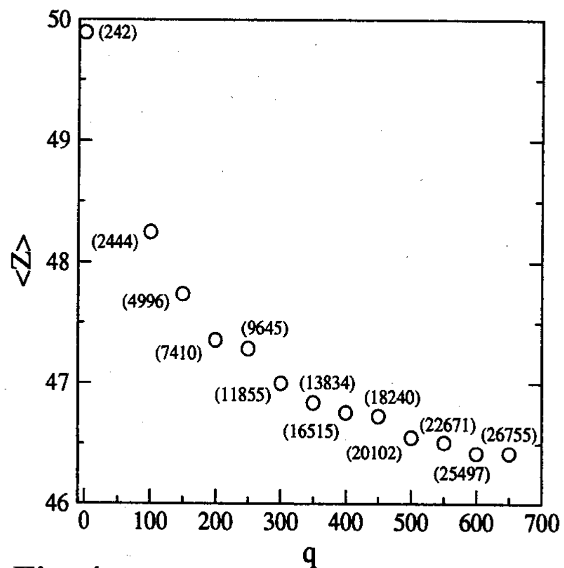

Fig. 4 Average ionization of Gold plasma Te = 2500 eV, Ne = 10^{12} cm^{-3}

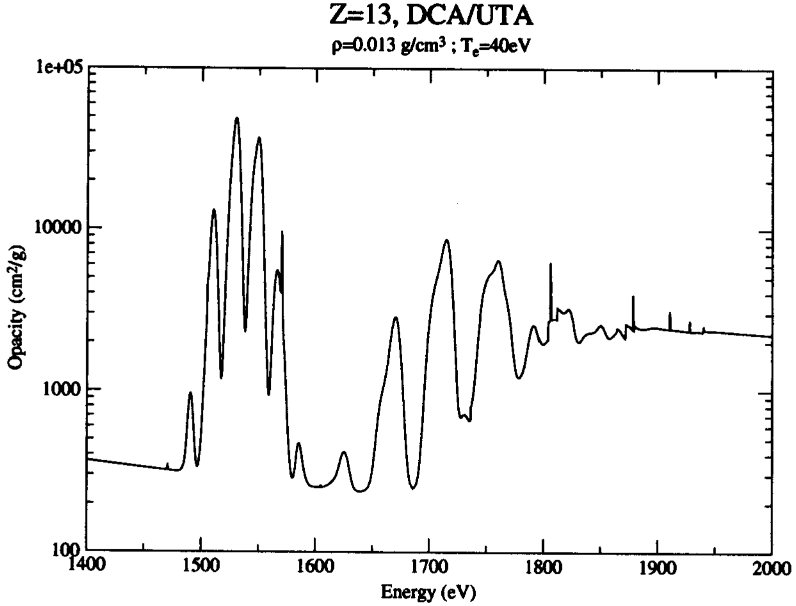

Fig. 5 K-shell opacity of an Aluminium plasma. Calculation using UTAs.

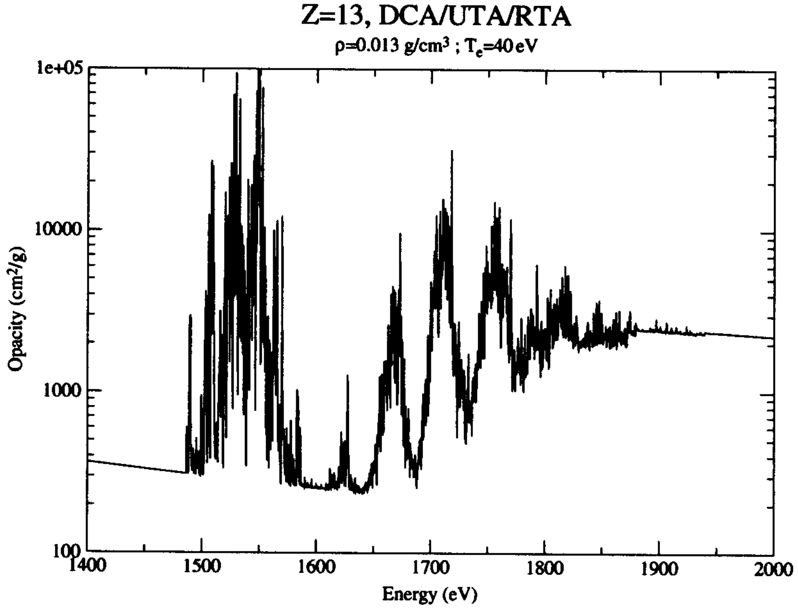

Fig. 6 K-shell opacity of an Aluminium plasma. Calculation using RTAs.

References

[1] O. Peyrusse, *Atomic configuration averages and non-LTE plasma spectroscopy calculations*, J. Phys. B **32**, 683 (1999).

[2] O. Peyrusse, *A superconfiguration model for broadband spectroscopy of non-LTE plasmas*, J. Phys. B **33,** 4303 (2000).

[3] J. Bauche et al. *Effective temperatures in hot dense plasmas*, J.Q.S.R.T. **99**, 55 (2006).

[4] O. Peyrusse et al. *Calculation of the charge state distribution of a highly ionized coronal Au plasma*, J. Phys. B **38,** L137 (2005).

[5] J. Bauche et al. *Transition Arrays in The Spectra of Ionized Atoms*, Adv. Atom. and Molec. Phys. **23**, 131 (1987).

[6] J. Bauche et al. *Analysis of a non-LTE xenon plasma by means of the model of superconfiguration temperatures*, J.Q.S.R.T. **81**, 47 (2003).

[7] F. Gilleron et al. *A statistical approach for simulating detailed-line spectra*, J. Phys. B **40**, 3057 (2007).

[8] Yu. Ralchenko et al. *Multi-Code Ab initio Calculation of Ionisation Distributions and Radiation Losses for Tungsten Tokamak Plasmas*, Proceedings of the 16th APiP Conference (in the press).