A Xenon Collisional-Radiative Model for Plasma Thruster Optical Diagnostics and Modeling

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Abstract: An extended Collisional-Radiative (C-R) model incorporating a significant amount of excitation levels, leading to the bulk of the Xe I to VII spectra, has been recently developed for diagnostics and modeling of Xenon plasmas. Among various other applications, this model is expected to significantly contribute to the optical diagnosis of the contemporary plasma thrusters and also allow for a correct analysis of their functioning.

Nomenclature

4CTMC	=	four body classical trajectory Monte Carlo code
$A_{i,j}$	=	transition probability, level *j* to *i*
ACE	=	atomic collisions with electrons code
CATS	=	Cowan atomic structure code
CbA	=	Coulomb approximation code

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C-R = collisional – radiative model
CTMC = classical-trajectory Monte-Carlo method
DW = distorted wave approximation
EIRENE = particle transport code
FAC = flexible atomic code
FOMBT = first order many body theory
GRASP = graphical representation and analysis of structural properties
l = orbital quantum number, $s = 0$, $p = 1$, $d = 2$, $f = 3$, …
LTE = local thermodynamic equilibrium
MCDF = multi-configuration Dirac-Fock
n = principal quantum number, here $n = 5, 6, 7, \ldots$
n_e = electronic density
RDW = relativistic distorted wave approximation
SPT-50 = prototype stationary plasma thrusters, 50 mm of diameter
T_e = electronic temperature
UV = ultraviolet spectral region
Xe I, II,.. = successive spectra of the xenon homo-nuclear sequence
Z = atomic number
λ = wavelength
σ_e = electron collision excitation cross section

I. Introduction

RADIATION emitted from various Xe plasmas, along with detailed Collisional-Radiative (C-R) models[1], can be used for developing optical diagnostics. Here we are specifically interested in the application of a C-R model for diagnostics and modeling of plasma thrusters fed with Xe. Such a model was previously developed[2] and applied to the study of two SPT-50 prototype devices[3] which were made available to us in the LPTP Laboratory of the Polytechnic school and in the ONERA Laboratory at Palaiseau[4]. The first of them was fed with either an Ar-Xe mixture or with pure Ar; it was then also diagnosed using an Ar C-R model[5]. Our earlier Xe model contained only the Xe I, II and III spectra and has been thoroughly validated for lower temperatures comparing with various experimental spectra.

Currently, there is a tendency to develop plasma thrusters reaching higher functioning temperatures, aiming to increase the thrust and to use the fuel more efficiently. In so doing, higher ionization stages of Xe are involved, requiring an extension of the number of ionization stages used in previous C-R models. We report here on such an extended model, able to take into account spectra from Xe I to Xe VII, which covers the entire range of population of the outer *p* shell of Xenon.

II. General Features of the Xenon Homo-nuclear Sequence

In the spectra of interest the resonant lines of the plasma, a significant part of the plasma radiation, are due to allowed transitions from the levels of the 6*s*, 7*s*, and 5*d*, 6*d*, 7*d* configurations which populate the levels of the 5*p* ground configurations. Depending on the ionization stage, the 5*d* ground level compound consists of one (Xe I, VII), two (Xe II, Xe VI) or five (Xe III, IV, V) levels. The successive ground level components are shown for neutral Xe and its first nine ionization stages in Fig. 1.

In the neutral Xe atom and all its ionization stages involving the external $5p^6$ electrons, there is a considerable number of metastable levels, either belonging to the *s* and *d* configurations when some of the $p - s$ and $p - d$ transitions, notably those concerning the 5*p* ground level compound, are forbidden, or because the entire *np* configurations cannot directly decay to the ground level configuration ($\Delta l = 0$). Besides, a number of transitions leading to $\Delta l > 1$ variations and transitions involving inner shells or doubly excited levels are present in the spectra of the successive Xe ions. A detailed work completed by E.B. Saloman on systematic evaluation of the Xe homo-nuclear sequence experimental spectra has been published lately and made available on line by NIST[6]. On can get an idea of the complexity of the excited levels structure from inspection of the two simplified Grotrian diagrams shown in the Figs. 2 and 3.

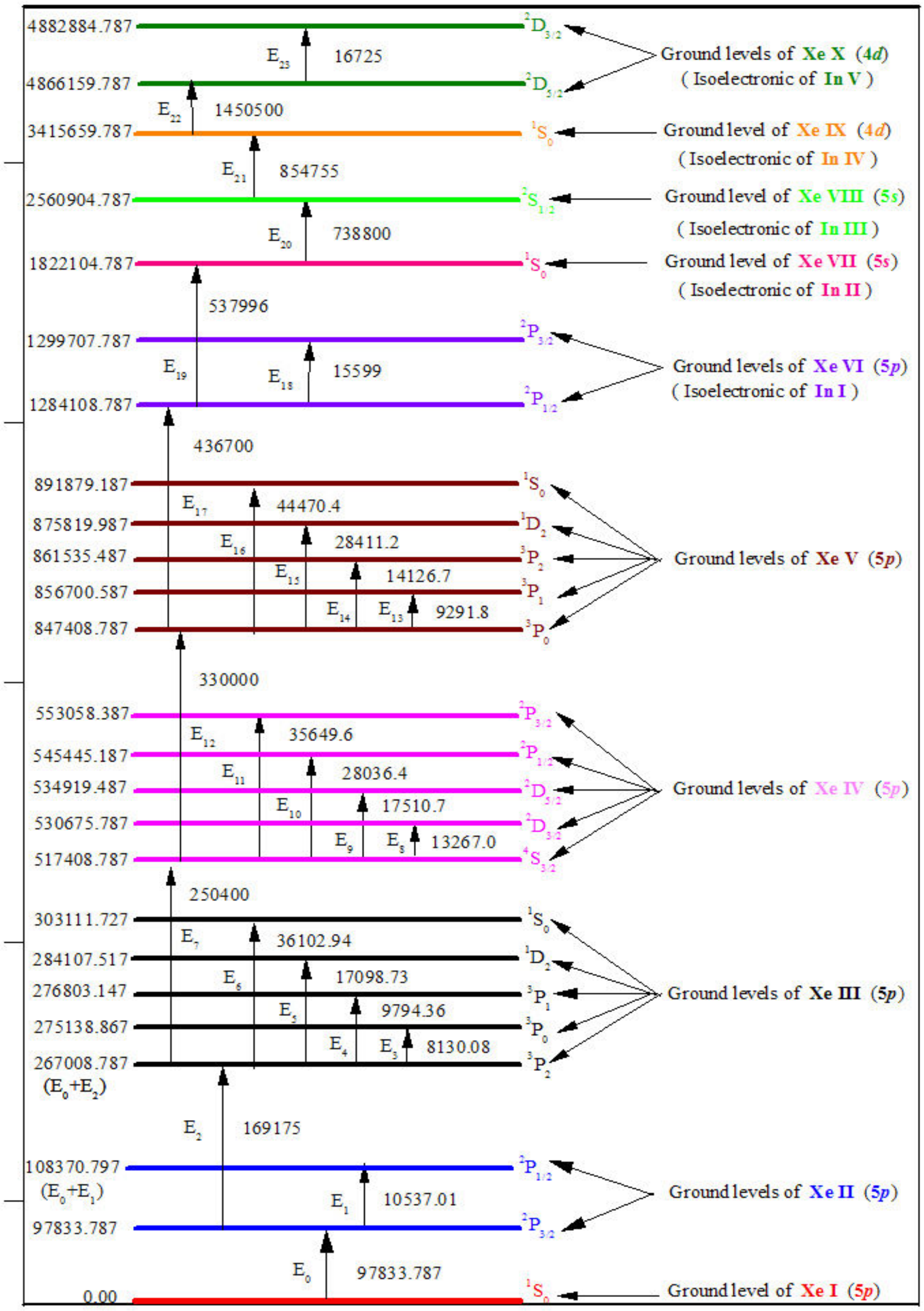
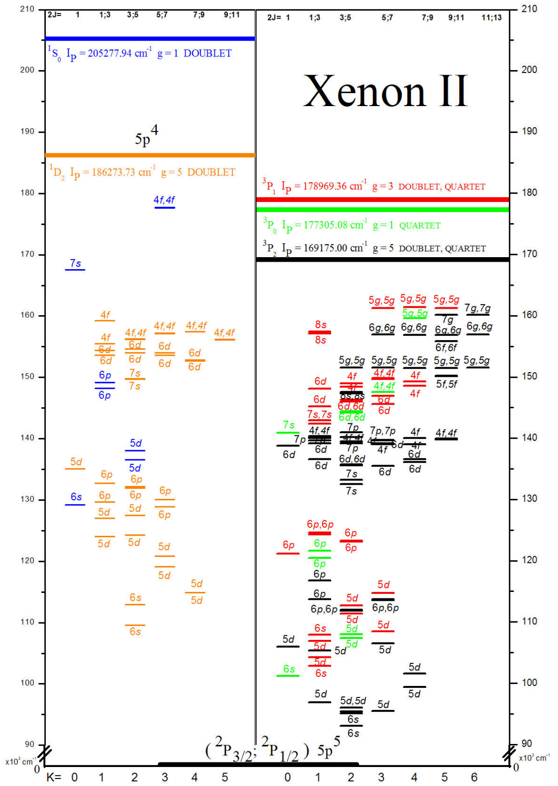


Figure 1. Ground levels compounds of the Xe I and its successive ionization stages up to Xe X.

Keep in mind that the resonant lines belong to a relatively constricted wavelength region in comparison with those coming from transitions between low lying multiplets. For the lowest ionization stages of Xe they appear mostly in the 50 to 200 nm UV region, while transitions between low lying excited states are mainly in the visible to infrared region, with the longest wavelengths corresponding to the neutral and for the lower ionized xenon species.



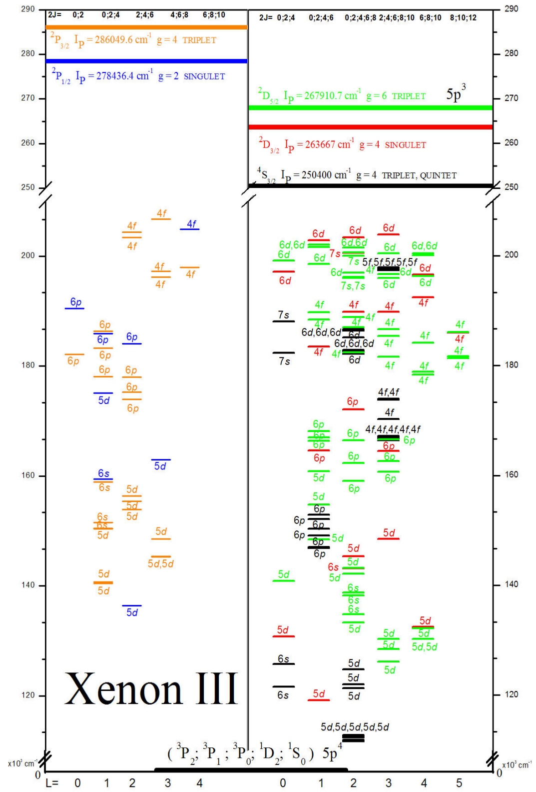


Figure 2. Simplified Grotrian diagram of Xe II.

Figure 3. Simplified Grotrian diagram of Xe III.

As a general trend, increasing of the ionization stage shifts the bulk of the spectrum towards the shorter wavelength region (UV, VUV) as it is expected empirically because the available energy has increased.

III. Calculation and Evaluation of the Atomic Data

Because the available experimental data are far from complete, we have used common theoretical codes in an effort to evaluate important atomic data for which no experimental data are available. We refer here to calculations of data used to determine spectral features of the neutral and of ionized Xe spectra, such as transition probabilities and electron collision excitation cross section.

The present atomic data evaluation is supported by work undertaken at the GAPHYOR Atomic Data Center of the LPGP Laboratory[7] in collaboration with the Atomic and Molecular Data Unit of the IAEA Nuclear Data Section, Vienna, and the LUTH Laboratory of the Observatory of Paris, Meudon. The data pertain to radiative and collision processes involving rare gases species, with emphasis placed on the study of low ionized Ar and Xe species. This work is part of an ongoing IAEA Coordinated Research Project[8] on *"Atomic data for heavy element impurities in fusion reactors"*. Evaluated atomic data produced by this project characterize the behaviour of the impurities encountered mainly in the edge (where the conditions may be comparable to those encountered in plasma thrusters) but occasionally in the core regions of fusion reactors, and cover both radiative (energy levels and transition probabilities) and collisional processes (involving electron and heavy particle collisions).

To further develop the evaluation of Xe atomic data we also rely on a collaborative work of GAPHYOR with the Laboratory of Computational Physics, Institut of Applied Physics and Computational Mathematics of Beijing currently in progress[9] with the goal of the evaluation of atomic data on structure, transition probabilities and excitation cross sections for high Z ions and of heavy particles collision processes. First priority is the assessment of atomic data for the Xe I to IX species, which will lead to a recommended data set to be used in C-R models applied to diagnostics and plasma modeling of Xe.

Experimental studies of A_{ij} for the Xe I, II and III multiplets, available in the literature, have been used throughout the evaluation work; use has also been made of recent experimental studies concerning higher ionization species[10, 11].

We present below the guidelines of some of the atomic data evaluation work, referring only to structure parameters, transition probabilities and excitation – de-excitation and ionization – recombination cross sections of the Xe species used in the present C-R model.

A. Structure Parameters and Transition Probabilities

Transition probability values for a number of Xe ion configurations[12] (including low radiative and metastable levels, and multiplets containing the most prominent lines in the Xe ion spectra) have been calculated using numerical codes based in well known theoretical methods:

1) CATS Code

We have made extensive use of the code CATS (Cowan Atomic Structure) which is part of the set of codes[13] developed at the Los Alamos National Laboratory (LANL), now available online. It calculates the transition probabilities[14] of the selected multiplet together with its atomic structure. This is an "ab initio" code, giving the possibility to select a list of configurations for a specified ion.

2) The SUPERSTRUCTURE Code

This code, developped by W. Eissner and collaborators[15], is currently used in Meudon Observatory for transition probability calculations.

3) The FAC Code

The Flexible Atomic Code (FAC) developed by Gu[16], has been installed at Meudon Observatory ; it calculates transition probabilities and excitation cross sections used for evaluation of the atomic data needed for our C-R model. Note that calculations of these atomic data in FAC are provided with construction of C-R models in mind.

4) Quasi-Classical Approximation

The code CbA based in the Coulomb Approximation[17], developed previously by K. Katsonis has been systematically used to obtain transition probabilities of multiplets belonging to neutral and ionized species of rare gazes, whenever experimental excitation energies are available.

5) The GRASP2 Package

Additional comparisons of the transition probabilities have been recently performed on the basis of calculations made with the GRASP2 package[18] in the relativistic multi-configuration Dirac-Fock (MCDF) approximation. Whenever the wavefunctions were sufficiently optimized, this code produced energy levels and transition probabilities often in satisfactory agreement with available experimental data, thus leading in principle to more realistic theoretical spectra[19].

B. Excitation – Desexcitation and Ionization - Recombination Cross Sections

To obtain correct theoretical spectra, an extended set of electron impact excitation cross sections is also required. We calculated these cross section mainly through the First Order Many Body Theory (FOMBT) and the Distorted Wave (DW) approximation using the code ACE[20] (Atomic Collision with Electron), also available at LANL. Some excitation data from the ground level and the metastable states have also been calculated using a quasi-classical CTMC code[21] and also a Relativistic Distorted Wave (RDW) code by R. Srivastava[22], especially for the Xe I species.

Excitation cross sections (σ_e) for the multiplets mentioned above containing allowed transitions were evaluated, but also for those containing only forbidden optical transitions. The latter are notably 5*p* – 6*p*, 7*p* and 5*d* – 6*d*, 7*d* for the Xe homo-nuclear sequence. The de-excitation cross sections have been always calculated from excitation using the principle of detailed balance.

These data, together with cross sections for ion-atom collision processes evaluated using 4CTMC, a four-body code resolving the four body Coulomb problem with the CTMC method[10], have been used in modeling and optical diagnostics of plasmas. Experiments for data validation include the UV region[11], where the resonance lines are expected to appear.

To complete the C-R model, evaluation of cross sections for various ionization and recombination processes was carried out as described elsewhere[4, 7], allowing for the determination of the dynamic equilibrium between the ionization stages included in the model. Photoionization cross sections, in principle of interest to reabsorbing plasmas, have been mainly used to obtain cross sections for radiative recombination on the basis of the detailed balance.

IV. Features of the Collisional - Radiative Model

Development of a detailed C-R model is necessary for the non intrusive optical emission diagnostics of the ionized Xe plasmas which are out of Local Thermodynamic Equilibrium (LTE), such as those encountered in electric propulsion. By means of such a model, information is also generated on the constituents and on most important processes encountered in the plasma. We have developed this model also because it can serve as the basis for a serious modeling of such plasmas, taking into account all of the ionized species, of which the multiply ionized are present in considerable percentages and cannot be ignored. On can get a measure of the relative importance of each ionic species by means of a simple coronal model of Xe[23] . For an electronic density of e.g. 10^{12} cm^{-3}, in an electronic temperature region of about 30 kK, where the Xe III spectrum is dominant with a Xe^{2+} relative abundance of about 60% , the Xe^{3+} stage is present with a relative abundance of about 30% and, although half the abundace of Xe^{2+} this stage carries a significant amount of the total positive charge because of the triple ionization (cf. 2x60=120 versus 3x30=90). Under the same plasma conditions, Xe^{1+} is expected to have a relative abundance not higher than 15% (and then 1x15 = 15), therefore carrying a positive charge amount six times smaller than the Xe^{3+} species. It is clearly that in this case it is a better approximation to neglect the Xe^{1+} rather than the Xe^{3+} species.

Furthermore, it is evident that to obtain a correct description of the bulk of the non-LTE plasmas, an extention of the “zero-dimension” C-R code to non-stationary and inhomogeneous plasmas is required. “Zero dimension” refers here to the fact that the C-R level populations expressed by the present status of the model are only locally valid. Resolution of the complete partial differential statistical equations system is hardly feasible and each time the left hand side of one statistical equation is set to zero the code is at most valid for the corresponding species only for a stationary state. Therefore we have previously proposed[2] to take into account the transport of all ion species with the code EIRENE[24], which was initially developed at the Institute für Plasmaphysik, Jülich, for modeling of Tokamak plasmas. For each species (here the Xe atom and its ions) the collisional radiative code needs to be compiled together with the EIRENE code before transport and atomic properties can be modeled in a consistent way. The study development begins with a very simple one dimensional slab, with spatial resolution in one direction only; energy is varying continuously and not in a discrete manner.

This type of integrated numerical experiment includes plasma physics, atomic and molecular processes and plasma-wall interaction. We are in the process of implementing our atomic model into this code.

V. Sample of the Calculated Theoretical Spectra Compared with Experimental ones

Detailed comparison of the theoretical spectra coming by the present model with those obtained experimentally, although giving a lot of information on the studied plasmas, is a cumbersome work which will be described elsewhere. A systematic experimental study of the Xe homo-nuclear series spectra is underway at the Organisme National d’Etudes et Recherches Aéronomiques (ONERA), at the Palaiseau campus. This study consists in registering emission spectra of a low density Xe plasma and determine the spectral lines belonging to the successive terms of the Xe homo-nuclear sequence beginning with Xe I. Here, we are restricted to summarily present only two typical cases of the C-R model applications, concerning two previous experiments. One of these experiments, of which the results have been published years ago[25] concerns mainly the visible region of the Xe I spectrum. Some data of the Xe II spectrum are also included. The second concerns spectra of the Xe II in the UV region, which have been registered recently and are on the way of being studied .

A. "Red" and "Blue" Lines of the Xe^0 Spectrum

We compare here the lines of the 6*s* - 6*p* multiplet of the Xe I spectrum provided by the present model with the corresponding lines of the standard experimental spectrum of Xe I given in the well known American Institute of Physics Handbook[25]. These lines, which are due to one excited electron among the six $5p^6$ external ones, are totally analogous to the well known "red lines" of the Ar I spectrum studied e.g. by a C-R model[26] using mostly the values of transition probabilities which one of us (KK) had compiled previously on the basis of the CbA code[27]. As can be seen on Fig. 4, the lines of the 6*s* – 6*p* multiplet according to the experiment[25] are slightly shifted towards larger wavelengths in comparison with those of the 4*s* – 4*p* multiplet of the Ar I given by a similar experiment[25]. This is in accordance with the shorter energy gap observed between the 6*s* and 6*p* configurations for the Xe atom. They still remain the stronger visible lines of the Xe I spectrum giving the reddish nuance to the spectrum and may be referred as "Xe I red lines". They are followed by the 6*p* – 6*d* lines which are also in the red region of the spectrum and also by the "blue lines" of the 6*s* – 7*p* multiplet, also shifted to larger

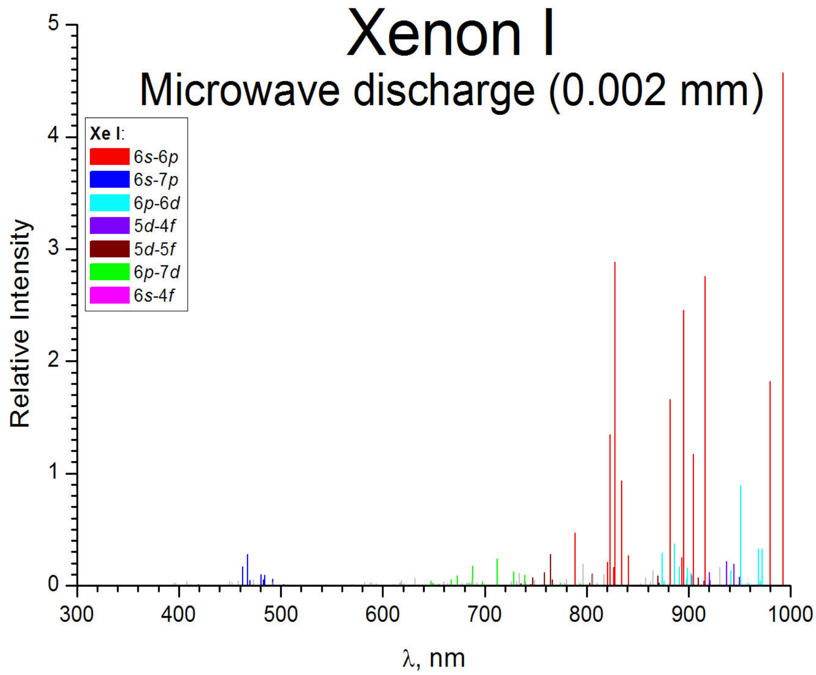


Figure 4. Experimental spectrum of Xe I (selected multiplets).

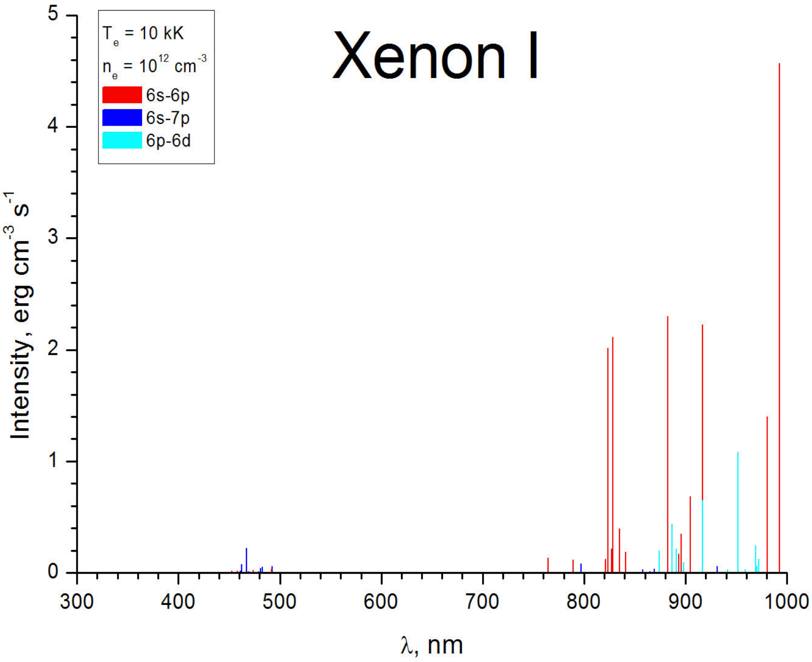


Figure 5. Theoretical spectrum of Xe I (C-R model, selected multiplets).

wavelengths, of which the bulk is situated approximately in the 440 nm – 500 nm spectral region, apart from their inter-combination lines which relate levels from different cores. In the American Institut of Physics Handbook, many spectral lines are registered. In fact, the Xe I table 7g-5 of the handbook, contains spectral lines which belong to the multiplets 5*d* – 4*f*, 5*d* – 5*f*, 6*p* – 7*d* and 6*s* – 4*f*. In addition to the 6*s* – 6*p*, 6*p* – 6*d* and 6*s* – 7*p* multiplets mentioned above. They are also contained in Fig. 4, but their intensity being relatively small, there are not easily distinguished. Therefore we have also made separate figures for each multiplet, not shown here, which contain even values taken directly from the experimental spectra of the figure 7g-4 and not included in the table 7g-5. The intensities of only the three main multiplet transitions of the total Xe I visible spectrum calculated by our code are given in the Fig. 5.

On the intensity of the resonant lines of the UV region, not shown here, we may observe that they can often be diminished because of the radiation re-absorption. Figs. 6 and 7 show specifically a comparison of the theoretical with the experimental spectra of the 6*s* – 6*p* "red lines" in the spectral region where most appear (750 nm to 1000 nm). The positions of the theoretical lines

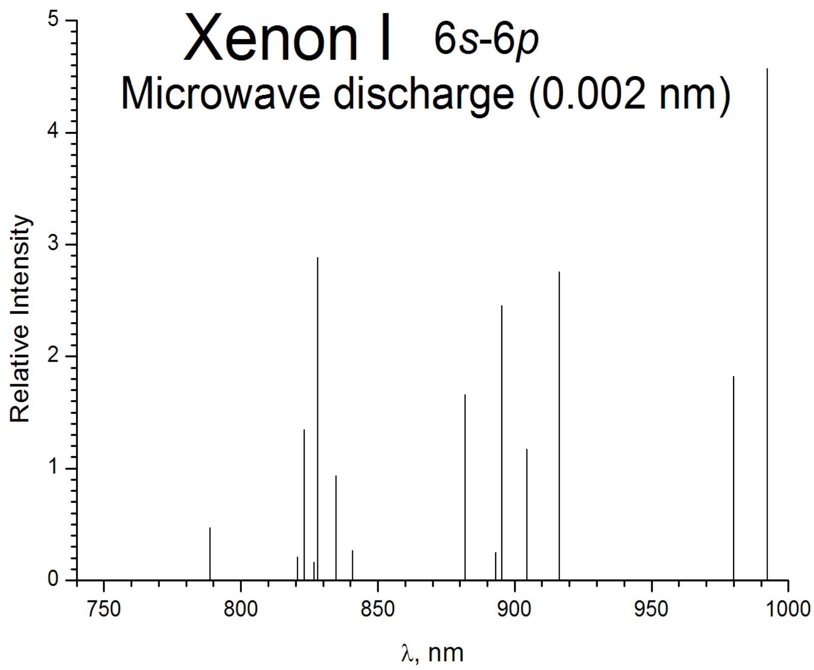


Figure 6. Partial (only 6*s* – 6*p* multiplet) experimental spectrum of Xe I.

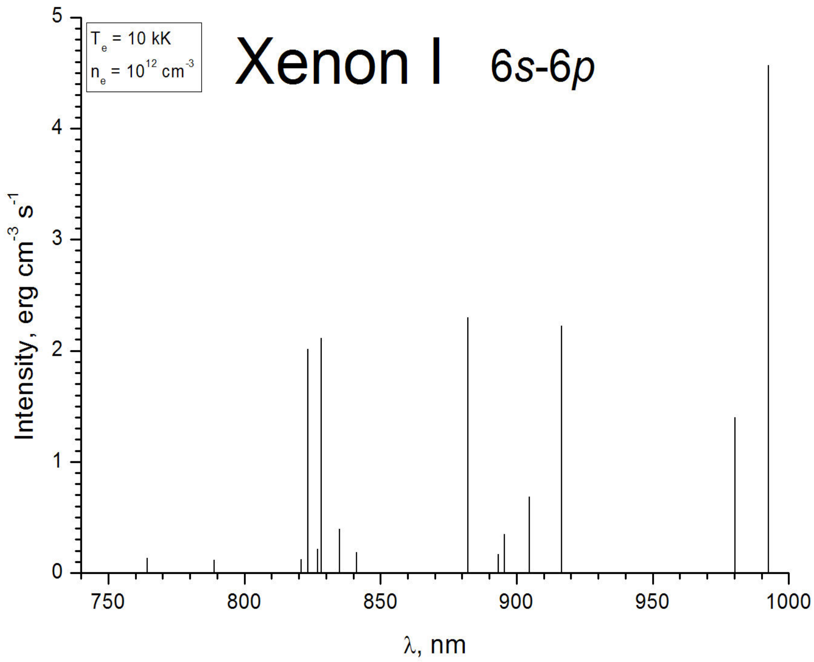


Figure 7. Partial (only 6*s* – 6*p* multiplet) C-R theoretical spectrum of Xe I.

agree well with the experimental line positions because the experimental values[6] have been used in the model in this case. There is a relative agreement between theoretical and experimental lines intensities for an electronic density n_e of 10^{12} cm^{-3} and an electronic temperature T_e of 10 kK. The observed differences may come from re-absorption and/or from the line of sight passing through regions with varying n_e and T_e, if the Aij and σ_e values are sufficiently well known (within, say, a 10% limit) and if the assumption of a single Maxwellian distribution function is approximately valid. Note that in Fig. 5 the calculated line intensities from our model are also shown for the 6*s* – 7*p* and 6*p* – 6*d* multiplets of a plasma at the same conditions n_e and T_e as before.

B. Resonant lines of the Xe II Spectrum

Let us now take an example from the Xe II spectrum resonant lines, of which the strongest are those coming from the 5*p* – 6*s* and 5*p* – 5*d* multiplets. Experimental study of the spectra emitted by low charge-state Xe ions requires both advanced experimental techniques for the confinement of the ions in conditions minimizing the collision effects and the sophisticated analysis of the observed spectra. To develop such a study, a 1 μA beam of Xe^+ ions was produced by the Van de Graaff accelerator IPNAS (Liege, Belgium) and subsequently passed through a thin carbon foil. After exiting the foil, the light emitted in the far UV by the excited ionized species was analyzed with a CCD-equipped spectrometer. Spectra of Xe in the 30-100 nm wavelength region have been recorded[11] at different beam energies, corresponding to different excitation energies. From the observed spectra, we present in Figs. 8 and 9 the lines belonging to the 5*p* – 6*s* and 5*p* – 5*d* multiplets (colored). Lines belonging to other multiplets and/or species are shown in gray color. The two figures contain lines in the 70 nm to 90 nm and in the 90 nm to 120 nm spectral region correspondingly. Figs. 10 and 11 show the theoretical results obtained by our model for an electronic density n_e of 10^{12} cm^{-3} and an electronic temperature T_e of 20 kK. Inspection of the four Figs. 8 to 11 leads to similar conclusions with those of the example A. As observed previously, the re-absorption of the resonant lines is in general expected to be larger, but we believe that its effect is minimized here because of the precautions taken in the experimental setup.

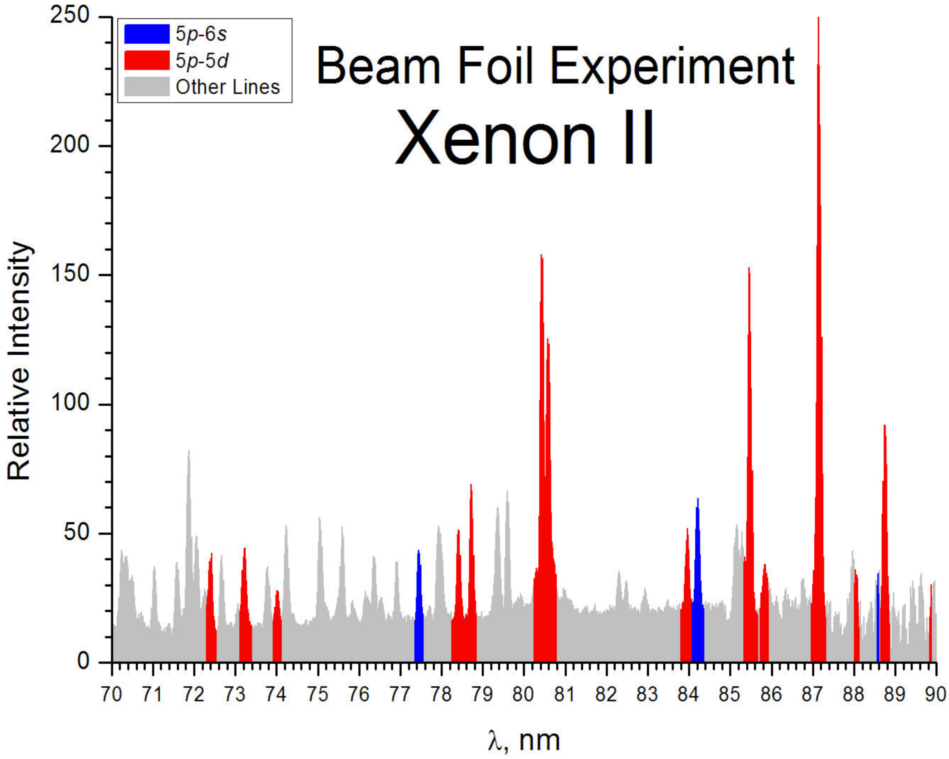


Figure 8. UV lines (colored) of the 5*p* – 6*s*,5*d* multiplets of Xe II.

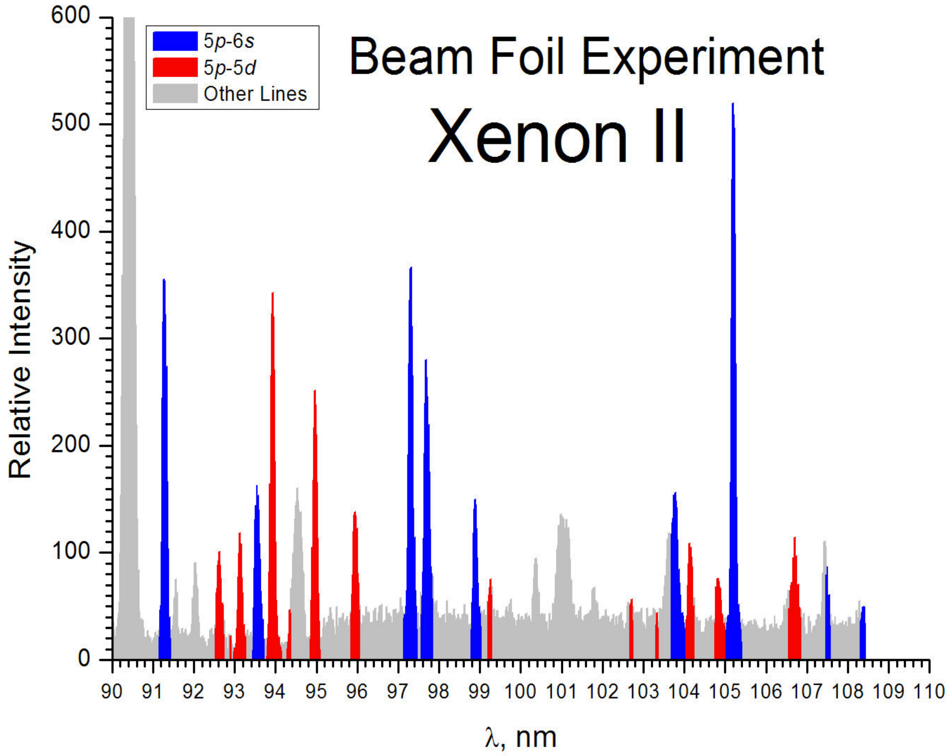


Figure 9. **As in Fig. 8.**

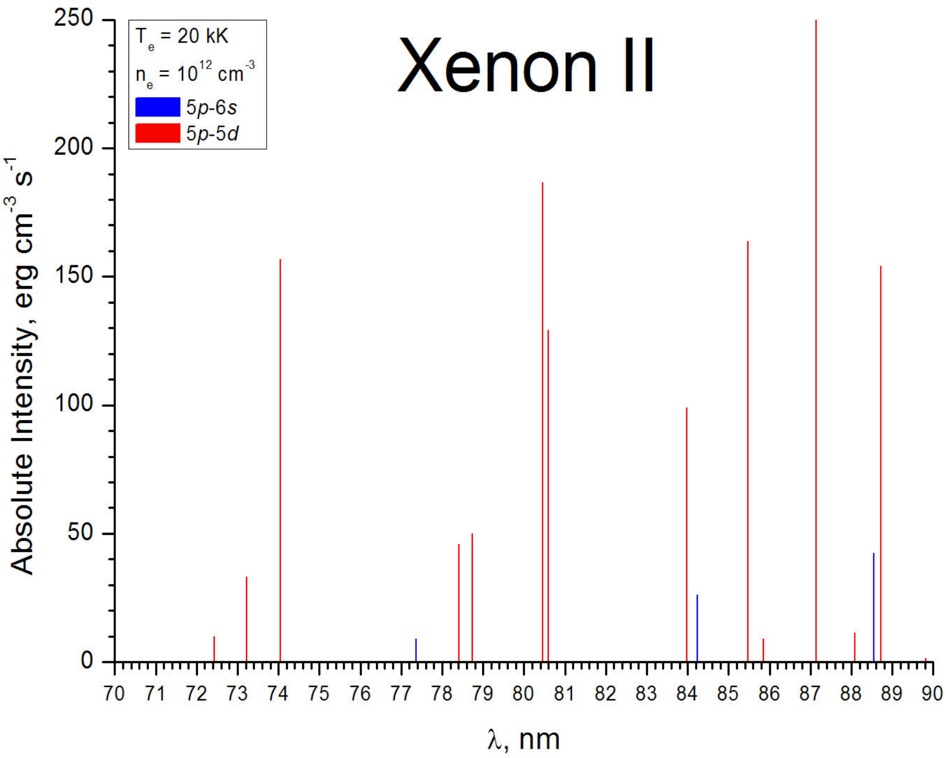


Figure 10. **Theoretical spectrum of the 5*p* – 6*s*,5*d* multiplet lines.**

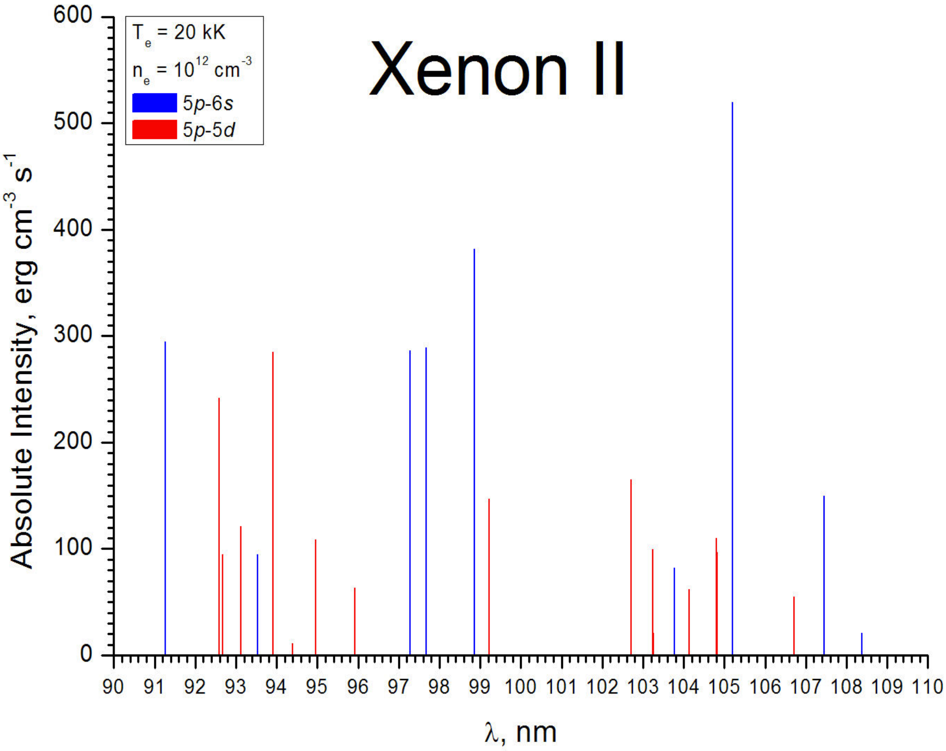


Figure 11. As in Fig. 10.

VI. Conclusion

A Collisional-Radiative model, taking into account the atomic properties of all the plasma constituents, allows for calculation of the parameters which are necessary for the local optical diagnostics. We describe the essentials of such a model which is a prerequisite for the detailed optical study of Xe plasmas, particularly of those present in plasma thrusters fed with Xe. This model, once coupled with a transport code, may lead to a realistic multi-dimensional model contributing to the study of various Xe plasma devices.

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