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Atomic Processes in Plasmas

Summary Report of Joint ICTP-IAEA School

Trieste, Italy

27 February – 3 March, 2017

Prepared by

H.-K. Chung and Yu. Ralchenko

June 2017

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ABSTRACT

This report summarizes the proceedings of the Joint ICTP-IAEA School on Atomic Processes in Plasmas. 56 participants from 19 Member States attended the event held at the Abdus Salam International Centre for Theoretical Physics (ICTP) in Trieste, Italy. The purpose of the School was to provide lectures, computer code training and information exchange for young students and early career plasma physicists, plasma spectroscopists, users of atomic data for fusion, astrophysics and laser and plasma applications, and atomic and molecular physicists interested in plasma spectroscopy to expand their knowledge of plasma spectroscopy and atomic processes in plasmas.

June 2017

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INTRODUCTION

The thermodynamic conditions of fusion plasmas, laboratory and industrial plasmas, laser-produced plasmas, astrophysical plasmas, and warm and hot dense matter are determined by numerous atomic processes including electron-ion and heavy particle collisions, photon-induced processes, and radiative decays. Even in fully ionized plasmas, which are typical for fusion energy research, atomic processes are very important in understanding plasma conditions as they underlie all impurity-based spectroscopic diagnostics.

The Abdus Salam International Centre for Theoretical Physics (ICTP) and the International Atomic Energy Agency (IAEA) jointly organized a school that was held at ICTP in Miramare, Trieste, Italy in the Giambiagi Lecture Hall of Adriatico Guest House, from 27 February to 3 March 2017. The purpose of the school was to provide young students and early career scientists in plasma physics communities with advanced training in theoretical and computational methods for atomic processes in plasmas. The school consisted of lectures by international experts, computer lab classes to learn state-of-the-art atomic codes, invited and contributed research talks, posters and discussion sessions, with good time available for personal interaction.

The previous advanced school and workshop on the similar scope were organized two years ago in 16-27 March 2015. Upon the suggestion from students of the 2015 school that the advanced school should be held regularly to educate and train young researchers in the field, the atomic and molecular data unit organize the school with more focus on the theoretical background of atomic physics and hands-on computer trainings. During the one-week school, 8 lecturers gave 9 lectures and 4 computer training classes for GRASP/RATIP, FAC, FLYCHK and CRETIN codes. The lecturers were C. Ballance (Queen's University Belfast, UK), H.-K. Chung (IAEA, Austria), S. Fritzsche (Helmholtz Institut Jena), H.-J. Kunze (Ruhr Universitat Bochum, Germany), Yu. Ralchenko (NIST, USA), H. A. Scott (LLNL, USA), J. F. Seely (Artep Inc, USA) and E. Stambulchik (Weizmann Institute of Sciences, Israel).

Thanks to the success of the previous school, there were many more skilled applicants than for the 2015 event. Highly qualified 56 Ph.D. students and early career researchers from 19 countries were selected from 191 applicants in diverse fields of fusion energy research, astrophysical science, laser-produced plasmas, atomic and molecular physics. Students presented their research posters on Monday afternoon and had numerous opportunities to discuss their results with fellow students and lecturers. The average age of students was 28 years old.

Proceedings of the school are summarized here. Appendix provides the school program, the list of participants and poster abstracts. Lecture materials, poster presentations from students are available at <https://www-amdis.iaea.org/Workshops/ICTP2017/> and selected lecture videos are available at <http://indico.ictp.it/event/7950/other-view?view=ictp timetable>.

PROCEEDINGS

The Advanced School started with welcome remarks from the directors. On the first day, lectures were provided in the topics of experimental spectroscopy by Prof. Kunze and atomic structure by Dr. Ralchenko. Experimental spectroscopy is one of the oldest and most important topics to learn in plasma studies. In recent years, not many universities teach experimental spectroscopy in classes and many plasma physicists should learn by self-study to perform their research. Therefore, this lecture on experimental spectroscopy provided a great introduction to the topic and references for further study. Atomic structure lectures provided fundamental basis on atomic processes and spectroscopic analysis. The poster session in the afternoon was highly beneficial for students to exchange their scientific knowledge and to get to know each other and lecturers. This kind of personal interaction among students and lecturers is an important factor and outcome of the school. Abstracts of posters are available in the Appendix.

On Tuesday, lectures were given on Radiation and Autoionization by Prof. Fritzsche, Collision Physics by Prof. Ballance in the morning and computer courses on GRASP/RATIP codes by Prof. Fritzsche in the afternoon. GRASP/RATIP codes are used to calculate atomic structure and transition probabilities. Many of students are not familiar with UNIX environment and therefore an introductory course on UNIX programming was offered in order to provide the basic information on how to run codes on UNIX environment.

On Wednesday, lectures continued on Line intensities and CR (collisional and radiative) modeling by Dr. Ralchenko and Radiation transport by Dr. Scott. In the afternoon, the computer course trainings for FAC (Flexible Atomic Codes) and FLYCHK were given by Dr. Stambulchik and Dr. Chung. The FAC code is a suite of atomic physics codes which provides necessary data sets to build a collisional radiative model for most plasma applications on atomic energy levels, radiative and autoionization transition probabilities, collisional excitation and ionization cross sections as well as photoionization cross sections. FLYCHK code calculates level population and ionization distributions over a wide variety of plasma conditions, and it is available at NIST (National Institute of Standards and Technology, USA). Both codes are widely used in plasma community for plasma diagnostics and spectroscopic analysis.

On Thursday, lectures continued on Line shapes by Dr. Stambulchik and Radiation transport by Dr. Scott. A short presentation on resources in plasma spectroscopy was given by Dr. Chung on IAEA atomic and molecular data unit's resources and by Dr. Ralchenko on NIST atomic data resources. In the afternoon, the computer training on CRETN code was given by Dr. Scott. CRETN code is a 3-D radiation transport code with a collisional-radiative model to provide spectroscopic intensity, emissivity and opacity for a plasma condition. The input and output formats are more complex than FAC or FLYCHK codes and the 2nd class on CRETN code was given on Friday afternoon.

On Friday, Dr. Seely gave a lecture on experimental spectroscopy, which was essentially an overview of practical applications of the methods covered during the week. Dr. Del Zanna gave a short presentation on CHIANTI database and programs widely used for solar physics and astronomy for low density coronal plasmas. The school certificates were handed out during a short question and answer session. At the end of the school a feedback form was collected. Responses were highly positive and the students suggested for such an event to be held regularly. Also, the students found the classes to be mostly at the reasonable level. The lecture materials are available at the Unit's webpage, www-amdis.iaea.org/Workshops/ICTP2015.

CONCLUSIONS AND RECOMMENDATIONS

Plasma spectroscopic diagnostics is the classic diagnostics technique used for more than 100 years in plasma physics. Lately, with the new and upgraded fusion and other plasma machines, the spectroscopic techniques are more important than ever. On the other hand, the new researchers in the field often do not have proper trainings in spectroscopic diagnostics or in atomic processes in plasmas. To help young and established researchers who are interested in these fields, the Joint ICTP-IAEA school on atomic processes in plasmas provided lectures and computer code trainings on various topics, from basic atomic physics to experimental spectroscopy to advanced collisional-radiative modelling. The second school in 2017 turned out to be as highly successful as the first school in 2015.

The collected feedback forms indicate that the students found the school very interesting, useful, and helpful. They appreciated the easy communication and valuable discussions with lecturers and stated that they were motivated with new ideas during the School. It was recommended that the School should be organized every year. Suggestions include: 1) lecture notes should be handed out before lectures, 2) computer labs could be longer or students may select computer labs, 3) at least 2 poster sessions should be open for more discussions, 4) more lectures on experimental techniques would be helpful, 5) a computer training course with realistic diagnostic cases using CR modelling, 6) some presentations on astrophysics or fusion plasmas for motivation, 7) parallel sessions with basic and advanced levels will be useful, 8) a clear set of notes on purpose or goal of computer training or group projects will be useful.

The organization by ICTP with Ms. Rosa del Rio and Dr. Joe Niemela was excellent. The computer room was large enough to accomodate 54 students in the class.

APPENDIX - Agenda

Monday, 27 February 2017

- 08:30 Registration and Administrative formalities 30' (Lower level (AGH))
- 09:00 Opening 50'
- 09:50 Break 10'
- 10:00 Experimental Spectroscopy 50'
- Speaker: Hans-Joachim Kunze (Ruhr Universitat, Bochum)
- 10:50 Coffee break 20' (AGH Cafeteria)
- 11:10 Experimental Spectroscopy 50'
- Speaker: Hans-Joachim Kunze (Ruhr Universitat, Bochum)
- 12:00 Lunch break 1h20' (AGH Cafeteria)
- 13:20 Atomic Structure 50'
- Speaker: Yuri Ralchenko (National Institute of Standards & Technology, Gaithersburg)
- 14:10 Break 10'
- 14:20 Atomic Structure 50'
- Speaker: Yuri Ralchenko (National Institute of Standards & Technology, Gaithersburg)
- 15:10 Coffee break 20' (AGH Cafeteria)
- 15:30 Poster Session 1h50' (AGH Lower Level)

Tuesday, 28 February 2017

- 09:00 Radiation and Autoionization 50'
- Speaker: Stephan Fritzsche (Helmholtz Institut, Jena)
- 09:50 Break 10'
- 10:00 Radiation and Autoionization 50'
- Speaker: Stephan Fritzsche (Helmholtz Institut, Jena)
- 10:50 Coffee break 20' (AGH Cafeteria)
- 11:10 Collision Physics 50'
- Speaker: Connor Ballance (Queen's University, Belfast)
- 12:00 Lunch break 1h20' (AGH Cafeteria)
- 13:20 Collision Physics 50'

Speaker: Connor Ballance (Queen's University, Belfast)

14:10 Break 10'

14:20 UNIX programming 50'

Speaker: Evgeny Stambulchik (the Weizmann Institute of Sciences, Rehovot)

15:10 Coffee break 20' (AGH Cafeteria)

15:30 GRASP/RATIP 1h50'

Speaker: Stephan Fritzsche (Helmholtz Institut, Jena)

Wednesday, 1 March 2017

09:00 Line intensities & CR modeling 50'

Speaker: Yuri Ralchenko (National Institute of Standards & Technology, Gaithersburg)

09:50 Break 10'

10:00 Line intensities & CR modeling 50'

Speaker: Yuri Ralchenko (National Institute of Standards & Technology, Gaithersburg)

10:50 Coffee break 20' (AGH Cafeteria)

11:10 Radiation transport 50'

Speaker: Howard Scott (Lawrence Livermore National Laboratory, Livermore)

12:00 Lunch break 1h20' (AGH Cafeteria)

13:20 FAC 1h50'

Speaker: Evgeny Stambulchik (the Weizmann Institute of Sciences, Rehovot)

15:10 Coffee break 20' (AGH Cafeteria)

15:30 FLYCHK 1h50'

Speaker: Hyun Kyung Chung (IAEA, Vienna)

Thursday, 2 March 2017

09:00 Line shapes 50'

Speaker: Evgeny Stambulchik (the Weizmann Institute of Sciences, Rehovot)

09:50 Break 10'

10:00 Line shapes 50'

Speaker: Evgeny Stambulchik (the Weizmann Institute of Sciences, Rehovot)

10:50 Coffee break 20' (AGH Cafeteria)

11:10 Radiation transport 50'

Speaker: Howard Scott (Lawrence Livermore National Laboratory, Livermore)

12:00 Lunch break 1h20' (AGH Cafeteria)

13:20 Resources in plasma spectroscopy 50'

14:10 Break 10'

14:20 UNIX programming 50'

Speaker: Howard Scott (Lawrence Livermore National Laboratory, Livermore)

15:10 Coffee break 20' (AGH Cafeteria)

15:30 CRETIN 1h50'

Speaker: Howard Scott (Lawrence Livermore National Laboratory, Livermore)

Friday, 3 March 2017

09:00 Experimental Spectroscopy 50'

Speaker: John F. Seely (Artep Inc., Ellicott City)

09:50 Break 10'

10:00 Experimental Spectroscopy 50'

Speaker: John F. Seely (Artep Inc., Ellicott City)

10:50 Coffee break 20' (AGH Cafeteria)

11:10 Q & A session 20'

11:30 CHIANTI Database and Programs 30'

Speaker: Giulio Del Zanna (University of Cambridge)

12:00 Lunch break 1h20' (AGH Cafeteria)

13:20 CRETIN 1h40'

Speaker: Howard Scott (Lawrence Livermore National Laboratory, Livermore)

15:00 Closing Session 30'



Joint ICTP-IAEA School on Atomic Processes in Plasmas

27/02/2017 - 03/03/2017

Trieste, Italy

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Joint ICTP-IAEA School on Atomic Processes in Plasmas

27 February – 3 March 2017

POSTER ABSTRACTS

In Alphabetical order of presenting participants

**Abdeltawwab Mohamed
Abrantes Richard June
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Anand Venu
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Bentotoche Mohamed Sadek
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Döhl Leonard
Dou Lijun
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Gao Lan
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Gruca Marta
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Jourdain Noémie
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Kostic Ana
Krušič Špela
Liu Liping
Liu Pengfei
Melsheimer Florian
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Pehlivan Asli
Priti Priti
Sereda Stepan
Shah Chintan
Sharma Prashant
Sheil John
Silwal Roshani
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Torretti Francesco
Vázquez Fernández Tello Elisa
Wan Yier
Wei Yanling
Wu Dong
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Comparative study on the mechanisms responsible for seed electrons generation in sodium plasma by LIBORS technique

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Abstract

Study is conducted to illustrate the physical mechanisms responsible for electrons generation in atomic sodium vapor using laser ionization based on resonance saturation (LIBORS) corresponding to the experimental conditions given by Farooq et al (**Farooq, Ahmad et al. 2001**). The analysis considered a sodium atom to be comprised of 22 levels such as a ground state, 18 excited states and three ionic states namely atomic, molecular and tri-atomic.

A modified numerical model (**Mahmoud and Gamal 1995**) is applied which involves the various collisional and radiative processes that might take place during the interaction. The model solves a set of equations which describe the rate of change of ground and excited states population beside three equations representing the rate of change of formed ionic states. In addition the model solves the time dependent Boltzmann equation for electron energy distribution function (EEDF) of the generated free electrons. A computer program is under taken which includes these mentioned equations as well as the relation who represents the cross sections and rate coefficient of the physical processes considered in this analysis.

The computations are devoted to analyze the individual effect of each ionization process responsible for generating the seed electrons required for electrons enhancement leading eventually to plasma formation. The results of computations of the EEDF, time evolution of the excited states population and ionic specific species formation for the individual effect of each ionizing process revealed that: the most effective processes are these resulting in the atomic photo-ionization, Penning ionization and electron impact ionization. On the other hand the density of molecular and tri-atomic ions producing during the interaction through associative ionization of atoms in the saturated energy state (3p-3p) and associative ionization of atoms in the 4d state and ground state molecules are found to be less effective in the comparison with the atomic ions.

Farooq, W. A., et al. (2001). Results on the laser ionization based on resonance saturation (LIBORS) in sodium vapor.

Mahmoud, M. A. and Y. E. E. Gamal (1995). "Modelling of Collisional Ionization in Laser Excited Sodium Atoms." Journal of the Physical Society of Japan **64**(12): 4653-4659.

Complexity Reduction of Atomic Collisional-Radiative Models

Richard Abrantes

Laser-plasma interactions are pervasive in the growing field of plasma physics. The increasing need to understand the physics in extreme conditions raises the demand for spectroscopic diagnostic tools that are capable of answering questions that conventional probes are unable to resolve. In order to correctly model the energy exchange and interpret the radiative signature from the plasma, one needs to accurately model the atomic state populations and the electron energy distribution function as well as their interactions with the radiation field. The most common approach is the Collisional-radiative (CR) model, which takes in account all the relevant atomic processes. The cost of such a detailed model is often prohibitive for multi-dimensional hydrodynamic calculations, yet simpler models are not sufficient. In this work, a reduction method for CR kinetics is discussed with a particular emphasis on time-accurate simulations.

The plasma kinetics being investigated in this work uses a comprehensive set of atomic data for argon from Los Alamos National Laboratory (LANL). Testing the full CR model also requires several processes to be modeled; in this framework, the processes include the electron-impact processes of excitation, deexcitation, ionization, and three-body recombination. Radiative processes have also been included in this work in the form of bound-bound radiation and bound-free radiation. The reduction method described in this work is based on the concept of grouping of levels. An internal distribution (uniform or Boltzmann) is assumed for all the levels within each group, and transition rates among groups can be determined straightforwardly by averaging over the group distribution. This leads to two reduction schemes: uniform and Boltzmann groupings.

The uniform grouping scheme groups a set of levels by weighing each level according to their respective degeneracy. The Boltzmann grouping scheme improves upon this by extrapolating a group temperature, maintaining a Boltzmann profile that is more accurate relative to the true solution. Various test cases conducted with these grouping schemes for a wide range of plasma conditions are shown, with implications leading to the coupling of the CR model with other solvers.

MCDHF calculations and study of plasma parameters for Li-like ions

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Abstract

Extensive configuration interaction calculations for several Ne-like ions ($Z=72-75$) are performed. we have reported multiconfiguration Dirac-Fock transition energies and wavefunction compositions of 209 levels belonging to the configurations $2p^5ns$ ($n=3,4,5,6,7$), $2p^5np$ ($n=3,4,5,6,7$), $2p^5nd$ ($n=3,4,5,6,7$), $2p^5nf$ ($n=4,5$), $2p^55g$, $2s2p^6ns$ ($n=3,4,5$), $2s2p^6np$ ($n=3,4,5$), $2s2p^6nd$ ($n=3,4,5$), $2s2p^6nf$ ($n=4,5$) and $2s2p^65g$ of Hf LXIII, Ta LXIV, W XV and Re LXVI. Radiative rates, oscillator strengths, transition wavelengths and line strengths have been calculated for all electric dipole (E1), magnetic dipole (M1), electric quadrupole (E2) and magnetic quadrupole (M2) transitions among these levels. These values were obtained using the GRASP (general-purpose relativistic atomic structure package) code which includes Breit and QED effects along with Dirac-Fock potential and second order coulomb interaction. We have compared our results with the data compiled using FAC (Flexible Atomic Code) and also with the recent results available in the literature. The accuracy of the data is assessed. Our calculated results are in good agreement with previous theoretical results and compiled values of the National Institute for Standards and Technology (NIST). We have also provided the line intensity ratios and plasma parameters for optically thin plasma. Our calculated data may be useful for experimentalists in identifying the fine-structure levels, for plasma modeling, astrophysical research applications.

PACS. 32.70.Cs Oscillator strengths, 32.10.Fn Fine and hyperfine structure

Abstract

Cold Atmospheric Plasma system can be considered as a viable method for Plasma Enhanced Chemical Vapor Deposition of thinfilms. The greatest advantage of this system is its vacuum free operation, which provides a cost effective alternative over conventional high vacuum systems. We have designed a reactor geometry for such a plasma system, in which, the contamination due to ambient air is minimized using as low a flow of Argon as possible. Towards this end, we have modeled and simulated the flow pattern of Argon gas entering the reactor geometry and have studied its effectiveness in removing air from the plasma zone. We have fabricated such a geometry and confirmed the findings of the simulation study through the experimental observation of the plasma optical emission. Further, we have studied the aspect of *filamentation* in atmospheric pressure plasma and have established the range of process parameters for which the plasma exists as a uniform glow. Subsequently, a complete system was developed, including an in-house built high voltage power supply, to generate a *Uniform, Contaminant free, Stable* plasma, suitable for thinfilm deposition over an area of 3" diameter.

- **Anand, V.**, Nair, A.R., Shivashankar, S.A. and Rao, G.M., 2015. Atmospheric pressure plasma chemical vapor deposition reactor for 100 mm wafers, optimized for minimum contamination at low gas flow rates. *Applied Physics Letters*, 107(9), p.094103.
<http://dx.doi.org/10.1063/1.4929781>
- **Anand, V.** and Gowravaram, M.R., 2009. On the purity of atmospheric glow-discharge plasma. *Plasma Science, IEEE Transactions on*, 37(9), pp.1811-1816.
<http://ieeexplore.ieee.org/stamp/stamp.jsp?arnumber=5175412>

We have also carried out Plasma Diagnosis, specifically to estimate the Electron Energy Distribution Function of the plasma, by analyzing the radiation emitted from an Argon plasma, acquired using an Optical Emission Spectroscope. The peaks in the spectrum were curve fitted with Voigt profiles and their FWHM and intensities were mapped to the electron number density and the electron energy distribution function of the plasma, using the mathematical models for Stark broadening and Corona population respectively. An optimization routine based on Nelder-Mead simplex algorithm was run to estimate the optimal values of these plasma parameters that produced a good match between the simulated spectrum and the experimentally acquired one. This analysis estimated that the value of electron number density in our plasma was in the range $0.82 \times 10^{17} \text{ cm}^{-3}$ to $3.56 \times 10^{17} \text{ cm}^{-3}$ and the electron temperature was in the range 0.36 eV to 0.39 eV. It also predicted that the EEDF closely approximated a Maxwellian distribution.

Thin film deposition was carried out as a means of proof of concept, using the newly fabricated system, by polymerizing Acetylene gas in the plasma to produce poly-acetylene films. The physical and chemical features of these films were studied using appropriate characterization tools and were compared with the findings of the process optimization studies. The films were doped with Iodine, for which a two order enhancement of conductivity was observed.

Shake-up processes in Auger Cascades of Light and Medium Elements

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In recent years, coincidence spectroscopy of photo and Auger electrons helped to investigate the de-excitation of atoms, molecules and solids. These techniques are, for example, used at synchrotrons to analyze the emission of multiple electrons due to Auger processes that follow the excitation or ionization of inner-shell electrons. The total kinetic energy of the emitted electrons allows to obtain information about the spectrum and population of the final states, while the individual electron energies reveal details about the intermediate states, and therefore the decay pathways of an Auger cascade.

To analyze such Auger cascade processes, we have extended the RATIP program [1], to model the multiple emission of electrons after creation of an inner-shell hole. Our studies reveal that many Auger cascades are strongly affected by shake-up (or down) transitions, in which the two-electron Auger process is accompanied by an additional (de-)excitation of a valence electron. For example, in the de-excitation of resonantly excited negative oxygen ions [2], complex electron correlation effects lead to a strong contribution of shake transitions to the total decay width. Furthermore, the population of higher lying intermediate states also enables the occurrence of three-step Auger cascade decays that are otherwise not possible due to energetic reasons.

The same effect was also observed in the two-step cascade that follows upon the photo ionization of a 4s or 4p electron of atomic cadmium [3]. Figure 1 displays the computed and experimental final-state spectrum of Cd^{3+} . In the lower part of the figure, the full spectrum is shown, while it's computed and measured population is shown in the upper panel.

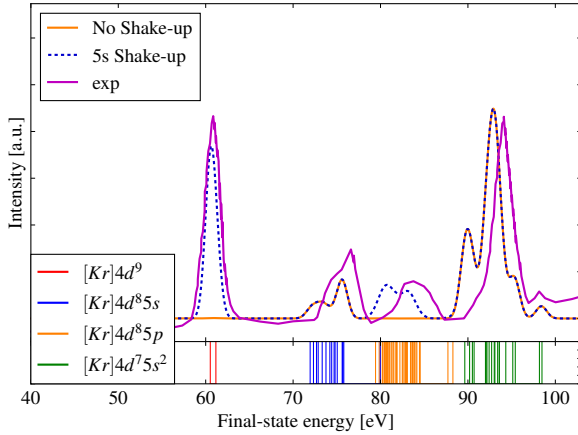


Figure 1: Computed and experimental final-state spectrum of triply-ionized cadmium. We consider a two-step Auger cascade that follows after photo ionization of a 4s or 4p electron in atomic cadmium. Shake-up transitions of a valence 5s electron are needed to explain the observed spectrum.

When the cascade formation is restricted to two-electron Auger processes, no shake-up transitions emerge and the yellow spectrum arises, where a significant portion of the observed population is missing. Taking shake-up transitions of the valence 5s electrons into account yields the dotted line, that is in very good agreement with experimental findings.

We will discuss the effects of shake-up transitions on Auger cascades of different elements and the theoretical models that are needed to account for the underlying electron correlation effects.

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Collisional-radiative calculations for the $J = 0-1$ lasing line of neon-like germanium under anisotropic excitation conditions

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Abstract. A new asymmetry parameter characterizing the differences between the polarized π and σ gain components of the soft-x-ray $J = 0-1$ lasing line of neon-like ions is calculated in the case of Ge^{22+} assuming an electron distribution which is a weighted sum of a Maxwellian isotropic and a monoenergetic beam. Using a steady-state collisional-radiative model, we determine in the weak amplification regime the populations of the upper $M = 0$ and lower $M = 0, \pm 1$ magnetic sublevels of the lasing line as a function of electron density from 10^{19} to $2 \times 10^{21} \text{ cm}^{-3}$. This model includes collisional excitation and de-excitation, as well as spontaneous radiative decay between all the 337 M -sublevels arising from the 75 lowest-lying Ge^{22+} J -levels. The computations were performed for a temperature T_e of the Maxwellian component between 1.2×10^6 and 8×10^6 K, a kinetic energy E_0 and a fraction f of the beam component in the ranges $1.5 - 20$ keV and $1 - 10\%$, respectively. The basic atomic data, such as level energies, radiative decay probabilities and collision strengths, were calculated with the flexible atomic code. However, some modifications of this code were made to get the collision strengths for transitions between M -sublevels due to impact with isotropic electrons as well as due to impact with an electron beam in the case of de-excitation. We find that the newly introduced asymmetry parameter may become significant under certain conditions of electron distribution corresponding to relatively low T_e ($1.2 \times 10^6 - 2 \times 10^6$ K) and E_0 ($1.5 - 4$ keV). The results reported here may be useful in the evaluation of the polarization degree of the $J = 0-1$ x-ray laser output from a germanium plasma in the presence of fast directional electrons.

Determination of the Composition and density gradients of the anode plasma in a relativistic-electron Diode using detailed shapes of continuum and line emission

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We analyzed visible spectra obtained in self-focusing, relativistic-electron diode experiments performed on an accelerator facility [1] at Sandia National Laboratories. An electron beam emitted from the cathode strikes a planar anode surface with high current densities ($\sim 1 \text{ MA/cm}^2$), forming a plasma on the electrodes that expands in the anode-cathode (A-K) gap. Radiation emitted from the plasma is imaged onto a spectrometer input slit via an optical fiber bundle. The spectrometer output is coupled to a streak camera, yielding spatially resolved and temporally resolved (5 ns) spectra. The spectra from the high-density plasma region mainly exhibit emission that appears to be continuum. However, the radiation intensity distribution cannot be explained by free-free or free-bound emissions. Rather, we suggest that the spectrum originates from blending of many Stark-broadened spectral lines. The analysis then allows for the use of the spectral intensity distribution to obtain quantitative and detailed information on the plasma composition, density gradients, velocities, and thermodynamic parameters.

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Temporal-spatially Resolved Measurement and Analysis of Extreme Ultraviolet Emission Spectra from Laser-produced Al Plasmas

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High-resolution spectral measurement for laser produced plasma is a powerful tool for studying the atomic structures of highly charged ions and radiation hydrodynamics in plasma. A clear understanding of evolution laws related to the ionization stages and plasma parameters in laser produced plasma is important for the construction of a spectral model in the field of astrophysics and laboratory plasma diagnostics and x-ray source applications.

In this work, a temporal-spatial resolved spectral measurement and analysis system of highly-charged ions from laser-produced plasmas is presented. And the corresponding semiautomatic computer software about measurement-control and spectral analysis has been written for achieving in best synchronicity required among the instruments, and avoiding a tedious comparative process between experimental spectra and theoretical simulated results. In order to demonstrate the capabilities of this system, a series of temporal-spatial resolved experiments of laser-produced Al plasmas have been also carried out. The results show that the system is a useful tool for studying the spectral structures of highly-charged ions and the temporal-spatial evolution behavior of laser-produced plasmas.

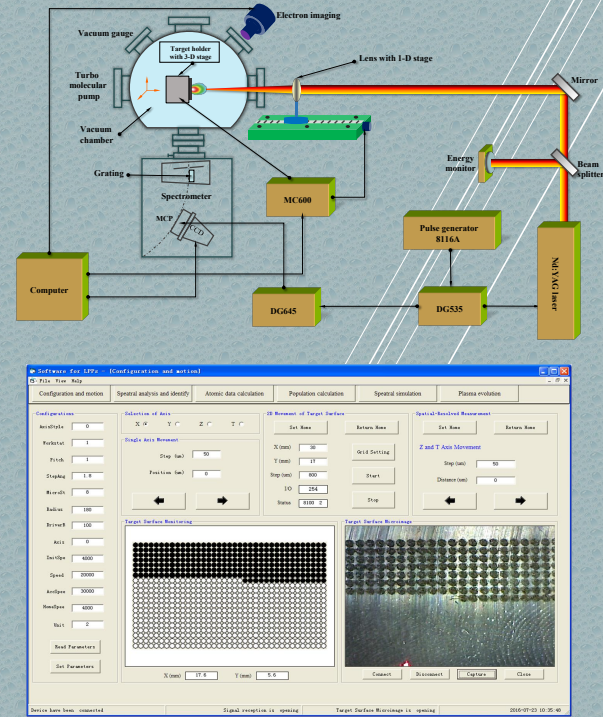


Fig. 1. Schematic drawing of the experimental setup and the interface of measurement-control and spectral analysis software of LPP.

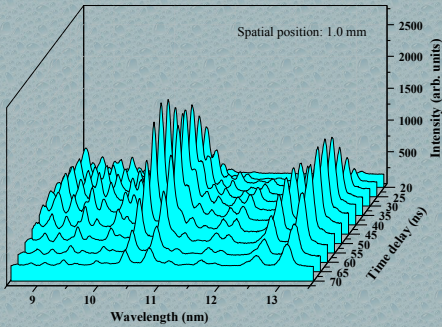


Fig. 2. Temporal evolution of EUV emission spectra from laser-produced Al plasmas.

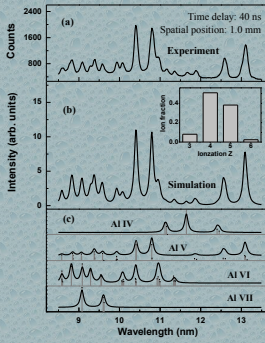


Fig. 3. Comparisons between the measured and simulated spectra.

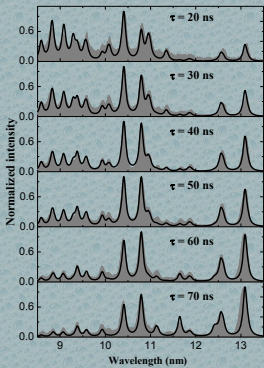


Fig. 4. Comparisons between the measured and simulated spectra for various time delays.

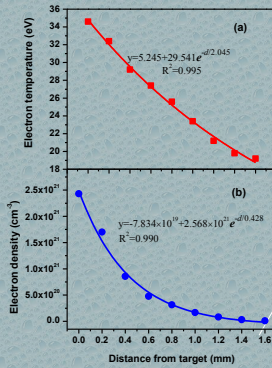


Fig. 6. Spatial behavior of electron temperature(a) and electron density(b).

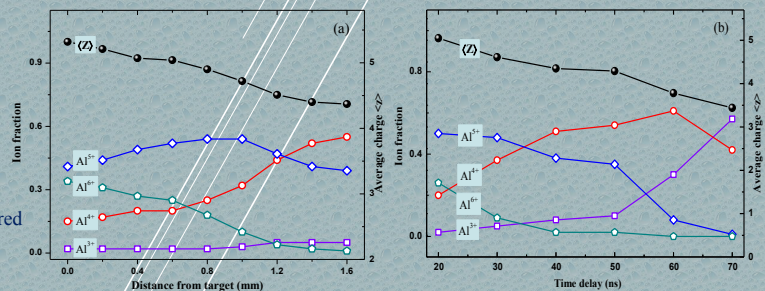


Fig. 5. Spatial and temporal behavior of the average charge $\langle Z \rangle$ and ion fractions of Al^{3+} to Al^{6+} ions.

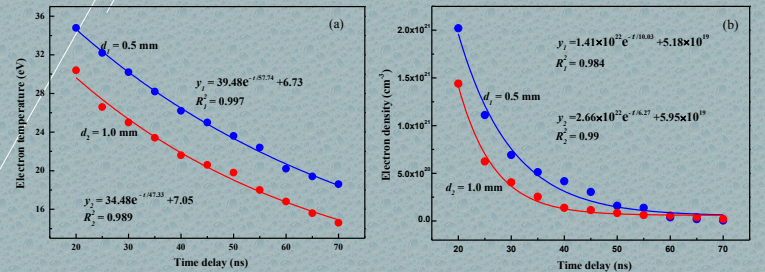


Fig. 7. The evolution of electron temperature(a) and electron density(b) with increasing time delay, at the distances of 0.5 mm and 1.0 mm from target surface.

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Improved classical description of $H(1s)$ and $H^*(n=2)$ for cross section calculations.

N. D. Cariatore

Abstract

An improved classical trajectory Monte Carlo (CTMC) methodology, specially conceived to provide a more accurate representation of the $H(1s)$ and $H^*(n = 2)$ targets, is introduced. Electron capture reactions from these targets by C^{6+} , N^{7+} and O^{8+} are used as benchmarks for the method. State selective cross sections are contrasted to those predicted by the standard microcanonical formulation of the CTMC method, the CTMC method with an energy variation of initial binding energies that produces an improved radial electron density, and the atomic orbital close coupling method. Present results are found in much better agreement with the quantal results than former formulations of the CTMC method.

X-ray and ion emission studies from laser produced plasma

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Laser produced plasma (LPP) is a brilliant source for X-ray and ion production. These LPP sources have various technical and scientific applications including inertial confinement fusion, X-ray microscopy, lithography, ion-driven fast ignition etc. Optimization of these X-ray and ion sources is important in order to obtain desired information and to find conversion efficiency as large as possible. In our lab, we have developed various laser systems such as 30 J/500 ps Nd: Glass laser, 2J/ 8ns Nd: YAG laser and 1 J/1ps Nd: Glass laser along with various plasma diagnostics such as X-ray diode arrays, X-ray crystal spectrometer, ion collectors, Thomson Parabola and optical shadowgraphy system etc. Using these facilities, we have conducted various experiments which will be discussed briefly in the next section.

In the first experiment, we have studied the X-ray and ion emission from Al plasma. The effect of varying the laser intensity on the emissivity of the K-shell resonance lines is found to follow a power law, $E \propto I^\alpha$ with $\alpha=2.2, 2.3, 2.4$ for He_β , He_γ , He_δ respectively. The temperature is estimated by taking the ratio of the Li-like satellite ($1s^2p-1s2p3p$) and the He_β ($1s^2-1s3p$) resonance line and the ratio of the He-like satellite ($1s2p-2p^2$) and the Ly_α ($1s-2p$) resonance line and is found to be 260-419 eV. Plasma density is calculated using stark broadening of the Ly_β spectral line and is found to be $5 \times 10^{20} \text{ cm}^{-3}$. These results are also verified by doing simulation using FLYCHK software. Angular distribution with respect to target normal for k-shell resonance lines and all charge states of Al ions is also analyzed. In our second experiment, in order to enhance the X-ray emission we have used SiO_2 foam with densities 50mg/cc and 70mg/cc, chromium doped SiO_2 foam along with solid Quartz. The X-ray and ion spectra are compared with the spectrum produced by solid Quartz. We found a two fold enhancement in soft X-rays flux in case of foam targets as compared to solid quartz and a decrease in hard X-rays is noticed from foam targets. This is due the fact that in case of foam targets, the volume of foam target irradiated with laser is higher due to electrom thermalization process and hence produce more soft X-ray yield than solid target, same can be seen from the shadowgraphy images where the X-ray emitting region is higher in foam targets than solid targets. In my presentation, we will discuss it in detail.

Simulation on charge states evolution of XFEL heated target

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Since X-ray Free-Electron Lasers (XFELs) give us a new opportunity to study x-ray—matter interactions, there have been several experimental results of nonlinear optical phenomena in the soft and hard X-ray regions at XFEL facilities. One of the interesting phenomena we want to present is the initial phase of transformation of solid density aluminum plasma by analyzing time-resolved extreme ultraviolet (XUV) absorption spectroscopy with a time resolution of 10 fs or less. XFEL generates the dense plasma state via K-shell photo-absorption and the properties of dense plasmas were probed by a few fs XUV pulses at various delays. XUV absorption edges are closely related to ionization energies of core electrons (ex. Al L-level) and electron distributions at the continuum. In order to verify the mechanism, the collisional-population kinetic code SCFLY is used to model XFEL heating. We calculate the temporal evolution of charge states and temperature of 200 nm aluminum irradiated with 5 keV XFEL pulse of 10 fs duration. This calculation could show the ultrafast dynamics of inner-shell electrons, and electron thermalization during intense XFEL – matter interaction. Also, opacity of XUV and emission spectra were calculated to verify the charge state evolution.

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Alpha Particle Transport due to Inelastic Atomic Processes

C. F. Clauser and R. Farengo

Alpha particles transport due to charge changes in magnetized plasma is studied. We presented analytical calculations [1] and particle simulations that show that charge changing processes can significantly modify the transport of alpha particles in the pedestal-edge-SOL regions [2].

The numerical code calculates exact alpha particles trajectories and includes both elastic and inelastic collisions. The latter are introduced via a Monte Carlo type method, in which the probability of each atomic process is taken proportional to the corresponding collision frequency. The cross sections of these processes were obtained from an existing database [3] but it is clear that more, and more accurate, atomic data are needed. The code runs on Graphics Processing Units (GPUs), thus allowing calculations with a large number of particles in a short time using modest computational resources.

First of all, we employed a simple 1D model and only included the inelastic collision of alpha particles with plasma species, He^+ and neutral deuterium (both atomic and molecular) and helium. In this case, we show that diffusion produced by charge changes (*inelastic diffusion*) becomes relevant at the pedestal-edge-SOL regions. The simulations also show that gradients in the density of the plasma and cold species, which are large and opposite in the edge region, produce an inward flux of alpha particles. It is also important to note that due to the inward flux, the alpha particle density should be very low near the separatrix, which is the region where the confinement can be significantly affected by the toroidal field ripple and perturbations produced by ELM control coils.

On the other hand, we have incorporated a 2D ITER-like geometry and are studying how these effects can change the density profile of alpha particles and its flux towards the wall and the divertor. For this, we have included the energy loss by elastic collisions mentioned above. In this way, we are studying the competition between these two transport effects. The simulations suggest that the alpha particle flux towards the first-wall components (wall and divertor) is substantially reduced by the inward flux, and thus a pedestal formation may appear due to this effect.

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Studies of high-resolution $K\alpha$ emission induced by suprathermal electrons generated by LULI2000 kJ-laser interacting with copper

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Suprathermal electrons generated by high-energy lasers is a key subject in the study of laser matter interaction with important applications in atomic physics and fusion science.

Although K_α X-ray emission at low spectral resolution ($\lambda/\delta\lambda > 500$) has routinely been applied to detect hot electrons a persisting key difficulty is the understanding of the K_α emission from near solid density but partially ionized (heated) matter of mid-Z-elements (like e.g., copper, iron) where open 3s-, 3p- and 3d-shell configurations have important impact.

We report here on the copper K_α -group emission near 8 keV and an experimental study conducted at the ps, kJ laser facility LULI2000, Palaiseau, France. Thin copper foils have been irradiated with 1 ω pulses. Two spherically bent quartz Bragg crystal spectrometers with high spectral ($\lambda/\delta\lambda > 5000$) and spatial resolution have been set up simultaneously to achieve a high level of confidence in the spectral distribution. In particular, we discuss the spectral distribution of open 3d-shell configurations where negative screening is predicted by multi-configuration Hartree-Fock atomic structure calculations. Finally we discuss possible implications for the analysis of non-equilibrium phenomena and present first atomic physics simulations.

H- and He-like Charge-Exchange Induced X-ray Emission due to Ion Collisions with H, He, and H₂

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The fundamental collisional process of charge exchange (CX) has been established as a primary source of X-ray emission from the heliosphere [1], planetary exospheres [2], supernova remnants [3,4] and starburst galaxies [5,6]. In this process, X-ray emission results from the capture of an electron by a highly charged ion from a neutral atom or molecule,

$$A^{q+} + B \rightarrow A^{(q-1)+}(nl^{2S+1}L) + B^+, \quad (1)$$

to form a highly-excited, high charge state ion $A^{(q-1)+}(nl^{2S+1}L)$. As the electron cascades down to the lowest energy level, photons are emitted, including X-rays. To accurately model the X-ray emission spectra and hence better understand the dynamics of these environments, it is essential to include the dominant collisional processes, including CX, for different ion and neutral interactions.

To provide reliable CX-induced X-ray spectral models to realistically simulate these environments, line ratios and spectra are computed using theoretical cross-sections obtained with the multi-channel Landau-Zener, atomic-orbital close-coupling, classical trajectory Monte-Carlo, and quantum mechanical molecular-orbital close-coupling methods. Using these calculations, X-ray line ratios and spectra, as shown in Figure 1, will be presented for collisions of H and He-like C to Si with H, He, and H₂ as their neutral targets. A velocity-dependent X-ray emission model produced with these line ratios will be shown for the Cygnus Loop supernova remnant.

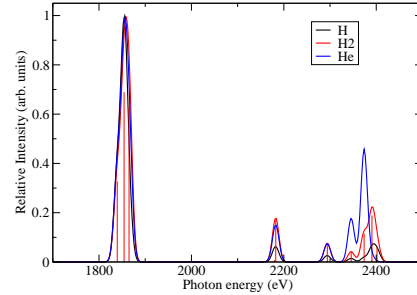


Figure 1: X-ray emission spectra and line ratios (for H₂) following the collision of Si¹³⁺ with H, H₂, and He at 1 keV/u (435 km/s). MCLZ cross-sections are used with a Gaussian resolution of 10 eV.

This work was performed in collaboration with David Lyons, Patrick Mullen, David Schultz, Phillp Stancil, and Robin Shelton. Work at UGA was partially supported by NASA grants NNX09AC46G and NNX13AF31G. Renata's research was supported by an appointment to the NASA Postdoctoral Program at the NASA Goddard Space Flight Center, administered by Universities Space Research Association under contract with NASA.

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Berry phase in plasma radiation theory

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Abstract

Using the adiabatic approximation (AA), we have derived the dipolar autocorrelation function (DACF) for Hydrogenlike atom in an adiabatically varying electric field. The DACF serves to compute the intensity of radiation in plasmas. The result is the emergence of the Berry phase in the expression of the intensity of spectral line in plasmas.

Introduction

In quantum mechanics, the adiabatic approximation corresponds to a time-dependent quantum system such as the perturbation undergoes large changes, but over a long period of time that the change in potential during the period of the light emitted in transition to the nearest neighboring state is small compared with the change of energy involved in this transition. The idea is that the quantum system always has time to adapt to environmental changes and passes through a succession of instantaneous equilibrium (and therefore instantaneous eigenstates). The adiabatic hypothesis assumes that the variations are slow enough, compared to the characteristic time of the transition rate, for a small number of instantaneous eigenvectors involved in the system description [1]. (this occurs for example in the problems in which we study the interaction of a molecule or an atom with radiation in a plasma submitted to external time dependent perturbation). In this work we shall use this hypothesis to evaluate the effect of an oscillating external electric field on the spectral line in plasma.

The Dipolar auto-correlation function

We start here by the time dipolar autocorrelation function of the radiator from which the spectral line shapes are generally deduced. The emitter is perturbed by ions and electrons treated as charged particles moving on classical paths [2]. For a description of the radiator-perturber interaction, it is usually sufficient to keep only the first term in the multipole expansion, using the so-called dipolar approximation. As quoted before, the effect of the electrons is usually treated with the impact theory by a collision operator. The electric microfield appearing in our formalism could thus be created by the electrons, the ions or both kind of particles. The usual start of spectral line shape theory is the general formula giving the radiation power :

$$I(\omega) = \frac{1}{\pi} \text{Re} \int_0^{\infty} C_{dd}(t) \exp(i\omega t) dt$$

In this formula $C_{dd}(t)$ is the autocorrelation function of the dipolar momentum of the emitter given by:

$$C_{dd}(t) = \sum_{\alpha\beta} \sum_{m=0,\pm 1} |d_{\alpha\beta}^{(0)}(\theta)|^2 \exp[i\gamma^{\alpha}(t) - \gamma^{\beta}(t)]$$

α and β are the upper and lower states respectively of the emitter and $d_{\alpha\beta}^{(0)}(\theta)$ are Wigner functions and

$$\begin{aligned} d_{\pm 1} &= Z e r_{\pm 1} \\ &= \mp Z \sqrt{\frac{1}{2}} (x \pm iy) \\ d_0 &= Z e r_0 \end{aligned}$$

are the electric dipole moment components with $r_{\pm,0}$ the standard position operators expressed in the spherical basis, and:

$$\gamma^{\alpha,\beta}(t) = \gamma^{\alpha,\beta}_D(t) + \gamma^{\alpha,\beta}_B(t)$$

Where $\gamma^{\alpha,\beta}_D(t)$ and $\gamma^{\alpha,\beta}_B(t)$ are respectively the dynamical and geometrical (Berry) phases relative to the states α and β [3, 4] :

$$\begin{aligned} \gamma^{\alpha,\beta}_D(t) &= \frac{i}{\hbar} \int_0^t E(F(t')) dt' \\ \gamma^{\alpha,\beta}_B(t) &= -m \Omega_B(t) \\ &= -m(1 - \cos \theta) \omega_0 t \end{aligned}$$

Application to the Lyman alpha line

So far we have calculated the Dipolar Auto-Correlation Function for an atom in an oscillating (rotating) electric field $\vec{F}(t) = \vec{f} + \vec{\varepsilon}(t)$. We can now apply this result on a plasma. Each atom in plasma is immersed in an electric field due to the plasma ions and the external electric field

$$\vec{\varepsilon}(t) = \varepsilon_0 (\cos \omega_0 t \vec{e}_x + \sin \omega_0 t \vec{e}_y)$$

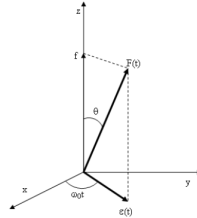


Figure B.1. The geometry of the rotating electric field in the plasma.

The frequency ω_0 must satisfy the adiabatic condition

$$\omega_0 \ll \left(\frac{3Zeaf}{\hbar} \right)$$

The DACF relative to the plasma is then obtained when making the average over the plasma electric field \vec{f} .

In the case of the Lyman alpha, we see that the Berry phase affects the two degenerate states; however the other two non-degenerate states are affected by Stark.

$$C_{dd}(t) = \frac{1}{3} \left(\langle 0 | \vec{d} | 2 \rangle \right)^2 \exp \left(-\frac{210.2}{\hbar} t \right) \left[\frac{f^2}{f^2 + \varepsilon_0^2} \cos \left(\frac{3\omega_0 f}{\hbar} t \right) + \frac{2\varepsilon_0^2}{f^2 + \varepsilon_0^2} \cos \left(1 - \frac{f}{\sqrt{f^2 + \varepsilon_0^2}} \right) \omega_0 t \right]$$

where $\vec{d} = e\vec{r}$ and $[\]_{\text{perturbers}}$ means that we must average over the perturbations represented by the electric microfield due to the ionic plasma component.

By inserting the effect of the electronic collisions by representing them with the collision operator ϕ_e in the intensity:

$$\begin{aligned} I(\omega) &= \frac{\phi_e}{3\pi^2} \frac{f^2 W(f)}{2(f^2 + \varepsilon_0^2)} \left[\frac{1}{\phi_e^2 + \left(\omega + \frac{3Zeaf}{\hbar} - \frac{10.22^2}{\hbar} \right)^2} + \frac{1}{\phi_e^2 + \left(\omega - \frac{3Zeaf}{\hbar} - \frac{10.22^2}{\hbar} \right)^2} \right] + \\ &+ \frac{\phi_e}{3\pi^2} \frac{f^2 W(f)}{2(f^2 + \varepsilon_0^2)} \left[\frac{1}{\phi_e^2 + \left(\omega + \varepsilon_0 - \frac{\omega_0 f}{\sqrt{f^2 + \varepsilon_0^2}} - \frac{10.22^2}{\hbar} \right)^2} + \frac{1}{\phi_e^2 + \left(\omega - \varepsilon_0 + \frac{\omega_0 f}{\sqrt{f^2 + \varepsilon_0^2}} - \frac{10.22^2}{\hbar} \right)^2} \right] \end{aligned}$$

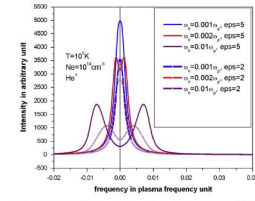


Fig. 2. Lyman- α lines in presence of rotating field with different strengths $\epsilon_0 = \epsilon$ and different rotating frequencies ω_0 at $T = 10^5$ K and $n_e = 10^{19} \text{ cm}^{-3}$.

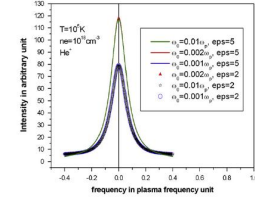


Fig. 3. Lyman- α lines in presence of rotating field with different strengths $\epsilon_0 = \epsilon$ and different rotating frequencies ω_0 at $T = 10^5$ K and $n_e = 10^{19} \text{ cm}^{-3}$.

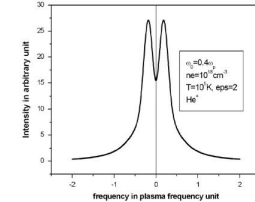


Fig. 4. Lyman- α lines in presence of rotating field with strength $\epsilon_0 = 2$ and rotating frequency $\omega_0 = 0.4\omega_0$ at $T = 10^5$ K and $n_e = 10^{19} \text{ cm}^{-3}$.

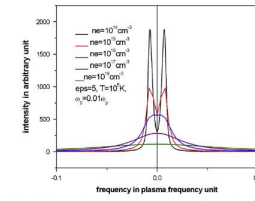


Fig. 5. Lyman- α lines in presence of rotating field with different densities at strength $\epsilon_0 = 5$ and rotating frequency $\omega_0 = 0.01\omega_0$ at $T = 10^5$ K.

Conclusion

When ω_0 decreases and reaches zero, the line becomes, as usual, broadened only by Stark effect whereas Berry effect is absent. But when increases, keeping of course (AA) criteria ($\omega_0 \ll \left(\frac{3Zeaf}{\hbar} \right)$), the Berry splitting appears at the center and the maximum of the intensity decreases. At the end, we note that we intend to generalize our findings when the rotation frequencies of the electric field become different and obeys to a given distribution.

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Possible explanation for the “Dark Matter X-ray line” at ~ 3.5 keV by charge exchange between S^{16+} and neutrals

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Speculations about a possible dark matter origin of a weak x-ray transition at ~ 3.5 keV have attracted enormous attention in the scientific community and given rise to a tide of publications attempting to explain the possible cause for this unidentified line-like feature. Cautiously, Gu and Kaastra et al. have pointed to a clear explanation for this phenomenon: charge exchange (CX) between bare sulfur S^{16+} and atomic hydrogen. By populating states in high principal quantum numbers n_{cx} of S^{16+} , the process drives a radiative cascade directly feeding the $n = n_{\text{cx}}$ to $n = 1$ transitions as well as other x-ray lines. Since S^{16+} and atomic hydrogen are present in the astrophysical objects where the 3.5 keV transition appears, an accurate model would be needed to scrutinize the relative intensity of the CX-fed transition. We approach the problem experimentally by breeding S^{16+} ions in FLASH-EBIT and keeping them magnetically confined with the electron beam turned off. During recombination of those ions with residual gas we collect x-ray spectra with a resolution of FWHM ~ 150 eV. By varying the production conditions we change the relative populations of the two ions of interest and distinguish their respective contributions. The 3.5 keV transition shows clearly up in the spectra under a wide variety of conditions and agrees with the astrophysical observations and the predictions of Gu and Kaastra.

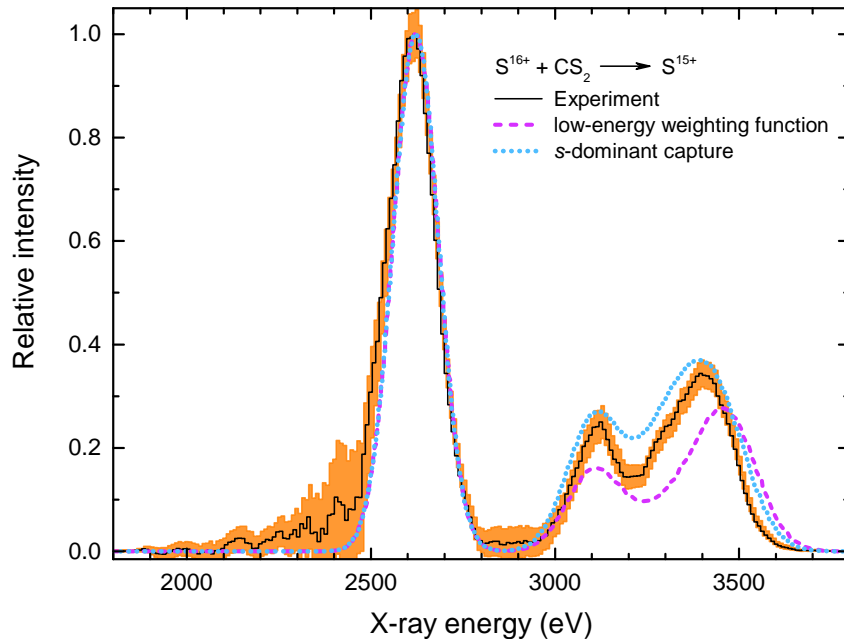


Figure 1: Comparison between experimental results and the model of Gu et al. of charge exchange between S^{16+} and CS_2 .

In-situ hollow ion spectroscopy of strong X-ray fields from ultra-intense laser-solid interactions

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Abstract:

Experiments at high power laser facilities, such as the Vulcan Petawatt Laser in UK, have observed the generation of hollow ions in low-Z micro-targets. The targets approach solid-densities in laser-solid interactions using a 10^{20} W/cm² high-contrast laser pulse. In-situ hollow ion spectroscopy infers that a powerful X-ray source, emerging as a consequence of the laser absorption coupling to fast electrons, must photo-pump these atomic states rapidly. Analysis of such X-ray spectra requires coupling analytical and modelling techniques to characterise the atomic kinetic and plasma physics. This methodologic approach would support future spectroscopic measurements to understand the physics of the system generating the intense X-ray field.

Theoretical Study of Dielectronic Recombination of Li-Like Xe⁵¹⁺ Ions

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Dielectronic recombination (DR) is a fundamental electron-ion collision process which is very important in astrophysical plasmas and in other natural as well as man-made plasmas [1]. It is also a powerful tool to investigate atomic ion structure to test the theoretical models and fundamental physics [2,3]. DR of Li-like ions has attracted much interest both in experimental and theoretical studies due to its simple structures in recent years [4]. In this report, the DR rate coefficients for the $\Delta n = 0$ transitions of Li-like Xe⁵¹⁺ (2s) ions are calculated using the flexible atomic code (FAC), in which the relativistic configuration interaction (RCI) method [5] was employed. The resonance energies, radiative and autoionization rates, and resonance strengths were calculated for the doubly excited states $(2p_{1/2}nl_j)_J$ ($n=18-32$) and $(2p_{3/2}n'l'_j)_J$ ($n'=9-27$) systematically. In combination with quantum defect theory (QDT) [6], the contributions from the high Rydberg resonance states with $n>32$ and $n'>27$ throughout to thresholds are obtained by extrapolation. Here l and l' values included up to 15.

Our calculated rate coefficients are compared with the experimental measurements at the heavy-ion storage ring ESR by Bernhardt et al [7], and a part of results for the $(2p_{1/2}18l_j)_J$ and $(2p_{3/2}9l_j)_J$ resonance manifolds is presented in Fig.1. Good agreement is obtained.

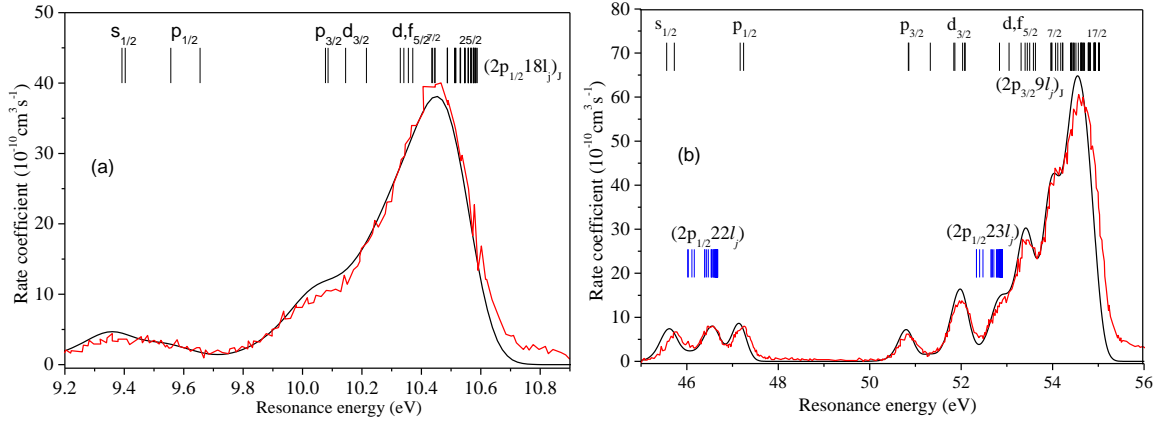


Fig. 1: Comparison of the present theoretical rate coefficients (black line) and experimental results (red line) for Xe⁵¹⁺ DR spectrum in the energy range of the $2s+e \rightarrow (2p_{1/2}18l_j)_J$ resonance (a) and $2s+e \rightarrow (2p_{3/2}9l_j)_J$ resonance groups (b), respectively. Vertical bars indicate the calculated resonance positions which shifted by -0.329 and -0.421 eV for the $(2p_{1/2}nl_j)_J$ and $(2p_{3/2}nl_j)_J$ groups, respectively. It should be noted that the $(2p_{3/2}9l_j)_J$ groups, which dominated at the resonance energy of 45-56 eV, are blended by $(2p_{1/2}nl_j)_J$ with $n = 22$ and $n = 23$ manifolds (blue vertical bars). The rate coefficients are obtained from the resonance strengths convoluted with 120 meV/k_B transverse temperatures and 0.2 meV/k_B longitudinal temperature.

The authors would like to thank C. Brandau for helpful discussions for the scaled resonance strengths. This work is partially supported by the National Natural Science Foundation of China (Grant Nos. U1331122, U1330117, U1332206, 11320101003, U1530142), and the External Cooperation Program of the CAS, No. GJHZ1305.

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ERO modelling of tungsten erosion in the linear plasma device PSI-2

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Erosion of plasma-facing materials, including tungsten (W), by high energy particles is one of the main problems in fusion research, in particular for future devices like ITER and DEMO. Linear plasma devices such as PSI-2 have a number of advantages for plasma-surface interaction (PSI) studies including continuous operation and small scale. However, numerical modelling is necessary for an understanding of the experimental observations and indispensable for the extrapolation of the obtained data to toroidal devices like ITER.

In this work, we use the 3D Monte-Carlo code ERO to simulate the PSI and local transport of impurities. The code ERO has been applied many times for predictive modelling of erosion/deposition and the impurity transport in ITER [1], as well as for earlier measurements at PSI-2 [2]. For the present contribution a number of code modifications were introduced such as the precise PSI-2 magnetic field configuration, diagnostics sightlines, 3D distribution of plasma density and temperature and target geometry.

A tungsten (W) erosion experiment was carried out recently in PSI-2 [3]. The experiment was conceived to provide a consistent set of data for the interpretation with the ERO code. In this experiment a rectangular W target with bias voltage applied to it was exposed to argon and neon plasmas with different conditions. W erosion was measured by three different methods: (i) spectroscopy along the installation axis to obtain the distribution of eroded W atoms in the plasma column; (ii) deposition measurements by means of a quartz micro-balance (QMB) diagnostic, positioned at various distances from the target to study the angular distribution of eroded W; (iii) spatially resolved weight loss measurements of the target.

Qualitatively the ERO simulations reproduce well all experimental dependencies: spectroscopy profiles, QMB measurements and weight loss. It was demonstrated that metastable tracking in ERO can explain deviations between modelled and observed axial WI intensity profiles for both neon and argon plasmas, demonstrating their strong influence on the W spectroscopy. Characteristic lifetime of WI metastable states was fitted as $t \approx 1 \cdot 10^{-5}$ s. The angular distribution of sputtered W atoms was determined by comparison of the modelled deposition on the QMB with the according experimental data and confirmed by additional molecular dynamics (MD) calculations. Erosion values were extracted from both experimental dependencies and ERO simulations. In general, our resulting sputtering yields are consistent with the SDTrimSP simulations.

The quantitative agreement is within 50% for all considered benchmark ERO applications but spectroscopy. WI emission intensity is by a factor of 5-6 higher than those observed with spectrometer in the experiment. These discrepancies are associated with uncertainties in the tungsten atomic data (PECs, ionization, recombination and collision rates). New photon emission data are already requested in ADAS. Other factors are possible deviations of electron velocities in the PSI-2 plasma from the Maxwellian distribution and flux alterations on the way from the Langmuir probe to the target due to recombination.

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Contribution of Lower Charge State Ar Ions to the Unknown Faint X-Ray Feature Found in the Stacked Spectrum of Galaxy Clusters

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Driven by the recent detection of an unidentified emission line previously reported at 3.55-3.57 keV in a stacked spectrum of galaxy clusters, we investigated the resonant dielectronic recombination (DR) process in Li-like Ar as a possible source of, or contributor to, the emission line. The Li-like transition $1s^22l-1s2l3l'$ was suggested to produce a 3.62 keV photon [1] near the unidentified line at 3.57 keV and was the primary focus of our study. The Electron Beam Ion Trap at NIST was used to produce and trap the highly-charged ions of argon. The energy of the quasi-monoenergetic electron beam was incremented in steps of 15 eV to scan over all of the Li-like Ar DR resonances. A Johann-type crystal spectrometer and a solid-state germanium detector were used to take x-ray measurements perpendicular to the electron beam. Our high-resolution spectra allowed the experimental separation of features that are less than 2 eV apart. We have used a collisional radiative model NOMAD [2] aided by atomic data calculations by FAC [3] to interpret our observations and account for the corrections and uncertainties. Experimental results were compared to the atomic database AtomDB, used to fit the galaxy cluster spectra. We find a number of measured features due to DR in lower charge state Ar ions not included in the database, close in energy to the identified line at 3.57 keV, and suggest their inclusion for improved interpretation and diagnosis of other astrophysical spectra.

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Simulation for radiative transfer of ultra-intense x-ray pulses through a solid-density aluminum plasma

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Radiative transfer of ultra-intense x-ray pulses through a solid-density aluminium sample is investigated theoretically by solving a one-dimensional radiative transfer equation. The laser beam is assumed to have a circle spot size with a Gaussian distribution of intensity and the time history of the laser pulse is also assumed a Gaussian profile. The pulse energy is 0.8 mJ with peak intensity of 1.24×10^{17} W/cm², duration of 40 fs (half width at half maximum), laser spot radial of 1.3 μ m and a bandwidth of 0.3%, respectively. Radiative transfer of such ultra-intense x-ray pulses through a 1 μ m thick aluminium sample is investigated. The populations of quantum states are obtained by solving a time-dependent rate equation based on collisional-radiative approximation[1-3], which are used to determine the absorption and emission coefficients of the aluminium sample. The produced free electrons are assumed instantaneously equilibrium to save the computational time. As an illustrative example, the population distribution and electron temperature of aluminium plasma irradiated by an x-ray pulse with photon energy of 1700 eV as well as the pulse shape through aluminium are discussed in detail. Then transmission of the ultra-intense x-ray pulses as a function of photon energy is calculated and compared with a recent experiment, where good agreement is found and saturable absorption is evidently observed. The transmission at a variable duration and laser spot size of x-ray pulses are also shown.

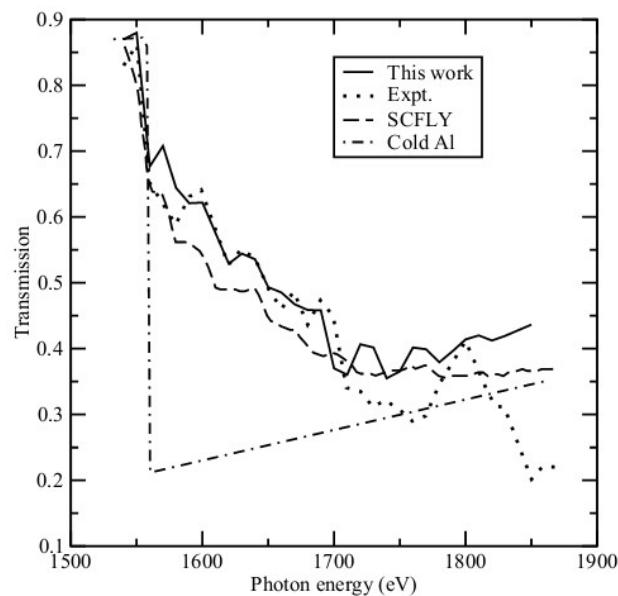


Fig.1 Transmission of x-ray pulses as a function of photon energy through solid-density aluminium: comparison with the experimental and other theoretical work [4].

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High-Resolution X-Ray Imaging Spectroscopy for High-Energy-Density Physics

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We have measured plasma parameters (T_e , T_i , and V_e) in magnetically confined plasma using high energy-resolution ($\lambda/\Delta\lambda > 5000$) x-ray spectroscopy for 3 decades. Recently we have been applying high energy-resolution x-ray spectroscopy to high energy density laser produced plasma: (1) an ultrafast spectrometer on the OMEGA EP Laser System at the Laboratory for Laser Energetics to measure Cu $K\alpha$ line shifts in rapidly heated targets [1]; (2) a spectrometer being built for the National Ignition Facility (NIF) at the Lawrence Livermore National Laboratory to measure hot spot electron density and temperature in an ignition capsule from Kr He α and He β spectra [2]; (3) a unique multi-cone crystal surface design for time-resolved measurements with a streak camera which – contrary to Hall’s traditional single-cone crystal spectrometer [3] - provides perfect imaging and high spectral resolution for an extended wavelength range [4]; and (4) μm -scale spatial resolution of a spherically bent crystal spectrometer at large magnifications [5]. For the two spectrometers on the OMEGA EP and NIF, details of the instrument design, preliminary experimental results, atomic physics calculations, and future experiments will be discussed. Also, lab testing, alignment and future applications of the two advanced spectrometer concepts will be described.

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Enhancing the predictive quality of laser-matter interaction simulations with PIconGPU via atomic model benchmarking

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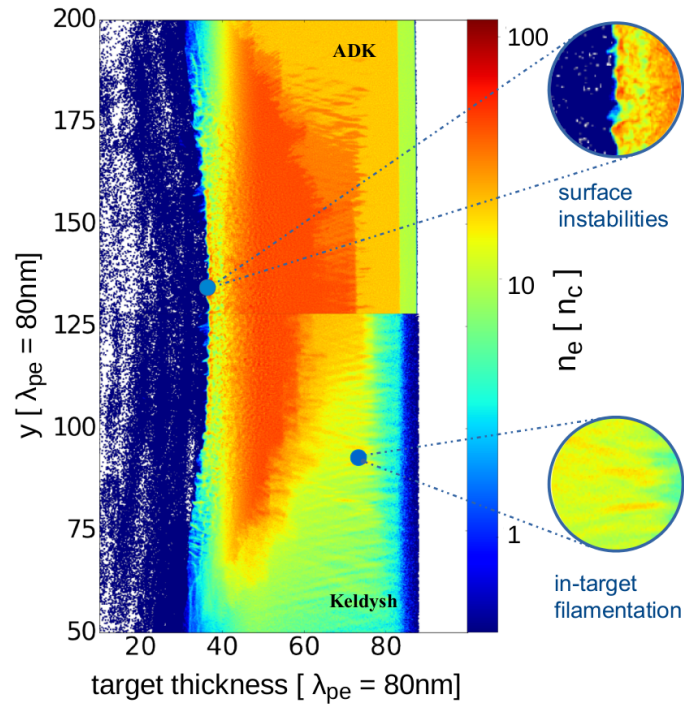
Technische Universität Dresden

In laser-generated plasmas the free electron density is a crucial parameter for plasma dynamics and for modeling its spatial and temporal evolution adequately, treatment of ionization processes is vital. In order to improve our understanding about the complexities of ultra-high power laser-matter interaction numerical simulations are an essential tool. There, we present a highly flexible framework for numerical field ionization methods implemented in the world's fastest 3D3V electromagnetic particle-in-cell code PIconGPU.

We will discuss various physical ionization models, compare them and show the methods we utilized to implement them effectively on GPGPU many-core architectures to manage the massively parallel Monte-Carlo processes of billions of particles per time-step.

In addition to this, the excellent scalability of PIconGPU allows for repeatable testing of the various ionization models against theory and between each other. Thus, computing a value for the systematic error is in reach and confidence can be created for the application of the code to complex setups like LWFA or TNSA.

Furthermore we have the opportunity to directly compare our simulations to laser-wakefield acceleration ionization-injection experiments that our laser-particle acceleration group is performing at the institute of radiation physics at the HZDR. With the outlook of upcoming experiments at HIBEF, the *Helmholtz International Beamline for Extreme Fields*, we also aim to give a range of validity for predictions of pump-probe experiments with high power lasers and X-ray free electron lasers.



Atomic structure calculations and study of plasma parameters of Al-like ions

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ABSTRACT

In the present work, the spectroscopic properties and plasma characteristics of Al-like ions (57-60) are investigated in an extensive and detailed manner by adopting GRASP package based on fully relativistic Multi-Configuration Dirac-Fock (MCDF) wave-functions. We have presented energy levels of lowest 148 levels for Al-like ions. We have also provided radiative data for electric dipole (E1), magnetic dipole (M1), electric quadrupole (E2) and magnetic quadrupole (M2) transitions for Al-like ions. We have also done a similar parallel calculation by employing fully relativistic distorted wave flexible atomic code (FAC) to check the reliability and authenticity of our results. Our calculated energy levels match well with our FAC results and other available results and we have discussed the discrepancies of our results with them. The variation of the line intensity ratio, electron density, plasma frequency and plasma skin depth with plasma temperature and nuclear charge are discussed graphically in detail for optically thin plasma in local thermodynamic equilibrium (LTE). We believe that our obtained results may be beneficial in future for comparisons and identification of spectral lines, in plasma modelling and in fusion and astrophysical plasma research.

Keywords: Energy levels, radiative data, transition wavelengths, Line intensity

Data analysis from the Pulse-Height Analysis diagnostic on Wendelstein 7-X stellarator

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The initial experiments devoted to optimization and tests of Wendelstein 7-X (W7-X) stellarator were conducted at the end of 2015. Helium and hydrogen were used as working gas. The Pulse Height Analysis (PHA) diagnostic, which was installed at W7-X, is the system which measures radiation from the plasma core in the energy range of 0.25 keV - 20 keV in order to estimate the electron temperature, identify plasma impurities and, if present, study of suprathermal electron tails. It can also provide the information to estimate line integrated Z_{eff} from measured spectrum.

The PHA diagnostic contains 3 energy channels equipped with Silicon Drift Detectors (SDD), which cover the whole energy range. The first and second channels are filtered with 8 μm of Be window to cover the energy range of 0.9-20 keV, while the third energy channel is covered by thin polymer window that allow to collect spectra between 250 eV and 20 keV. The temporal resolution of the PHA system is 100 ms.

In this paper the average electron temperature is estimated by distinguishing free-free radiation (*Bremsstrahlung*) in the spectrum and averaging over the acquisition time. Such an estimation of the temperature has been done for discharges in different experimental conditions and is occurred to be comparable to the results of averaged temperature obtained e.g. from Thomson scattering.

Another considered aspect was the identification of plasma impurities. After the first operational phase on W7-X (OP1.1) the spectral lines intensities are estimated by fitting Gauss function. For the following, identified spectral lines: S XV, S XVI, Cl XV, Cl XVII, Ar XVII and Ar XVIII such an approximation has been done.

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Current status of charge exchange research in astrophysical field

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Charge exchange (CX) is an emission mechanism newly introduced to X-ray astronomy. So far the most notable application of CX is to model the solar wind interactions with planets, comets, and the heliosphere [1]. Application of CX to extrasolar X-ray objects still remains rather speculative; most researchers still consider CX only as a foreground soft X-ray emission (solar wind interaction with the earth magnetosheath) for their objects. However, as we will show later, CX has an enormous potential in studying various objects, such as clusters of galaxies. There is a vast discovery space left to explore for CX, which may potentially make CX one of the future highlights of X-ray astronomy.

CX occurs when an ion collides with a neutral atom, and catches an electron from the atom. The resulting line emission is unique, since (1) it appears at energies that are very different from the thermal emission; (2) it is highly velocity-dependent. For a long time, CX study suffered from the lack of an accurate plasma emission code. In 2016, we published a ground-breaking plasma code dedicated to the CX X-ray modeling. For the first time, our model gives a successful fit of the high-resolution X-ray spectrum from comet C/2000 WM1 [2]. We can also model the CX in lower energies, e.g., UV, optical, and infrared bands, for interactions between lowly-ionized ions and atoms/molecules.

So far the most intriguing application of the CX model is the mysterious 3.5 keV line feature. In 2014, two groups reported to have detected a weak line feature at ~ 3.5 keV in the X-ray spectra of clusters of galaxies, which does not match with any known thermal line [3,4]. It immediately vitalized the astrophysical and particle physics communities, leading to ~ 300 follow-up journal papers, most of which discussed a possible origin that this line is created by radiative decay of sterile neutrinos known as a dark matter candidate. We are the first and only group pointing out that there is actually a more natural, alternative explanation to the line: CX emission by hot, fully-ionized sulfur ions colliding with cold, neutral atoms [5]. Recently, we have confirmed our theoretical calculations by laboratory measurements using an EBIT experiment [6].

The mysterious 3.5 keV line has been revisited recently by the newly-launched Hitomi satellite. As reported in the Hitomi collaboration paper [7], the expected “sterile neutrino line” is not found, instead, the predicted strength of the CX lines [5] agrees with a possible signal at $\sim 2\sigma$ level in a short-exposure Hitomi spectrum of the Perseus cluster. This is the first time that the characteristic CX line is detected, though very marginally, in galaxy clusters. Only our model was able to predict this. Our work opens a new window for studying CX in clusters.

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Electron impact ionization cross section of C_3F_x ($x=1-8$): useful data for plasma modeling

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Electron interaction with atoms and molecules play a fundamental role in understanding and modeling of atmospheric and industrial plasma. The electron-impact dissociation of the stable parent molecules such as CF_4 , C_2F_6 , C_3F_6 , C_3F_8 , C_4F_6 , and C_4F_8 in the plasma leads to the formation of reactive radicals C_xF_y ($x=1-3$, $y=1-7$) which are important for the chemical reactions in fluorocarbon-containing plasmas [1]. The ionization of parent molecules along with its daughter fragments and radicals is one of the important chemical reactions occurring in plasma. Among the C_3F_x ($x=1-8$) fluorocarbon species, only C_3F_6 and C_3F_8 are studied for ionization and there are no data for other targets. C_3F_8 is being extensively studied for ionization by many experimentalists and theoreticians and recommended values are also given by Christophorou and Olthoff [2]. However for C_3F_6 there is only one recent measurement of Bull et al [3] along with their binary-encounter Bethe (BEB) [4] calculation for ionization is available. The two results disagree among each other by 40%. Hence there is a need for more investigation for these systems along with other targets species for which there are no data in the literature.

In the present study we have used the BEB [4] method to calculate and study the ionization cross section (Q_{ion}) for all the targets. The various computational theories are employed for orbital energies and the Q_{ion} is investigated for all the targets of the series C_3F_x ($x=1-8$). All the species are optimized using Density Functional Theory [DFT (ω B97X-D)/aug-cc-pVTZ] and the calculation of orbital parameters with different level of approximation is done using the Gaussian 09 [5]. Our idea is to find the accurate values of the binding energy which is an important input for the BEB cross section. To get an idea about the uncertainty in the calculation, we need to investigate various levels of theories for the orbital parameters and have to generalize based on the accuracy of the binding energies. It is not just the energy of the highest occupied molecular orbital (HOMO) but the binding energy till 40 eV has to be very accurate for BEB cross section. We have obtained some interesting results for BEB cross section using the DFT (ω B97X) functional for orbital energies. Based on the results of the C_3F_x ($x=1-8$) and other targets species these issues will be discussed in the workshop.

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The Spectrum of Selenium Ions (Se I-III) from 300 Å-1500 nm: Ritz wavelength and Optimized Energy Levels.

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We report new measurements of selenium spectra, a member of iron group element detected in nearly twice as many planetary nebulae as any other trans-iron element. Current work includes comprehensive analysis of neutral, singly and doubly ionized (Se I, Se II, and Se III) in the vacuum ultraviolet (VUV) to infrared (IR) region. Theoretical predictions of level energies and transition probabilities in Se I-III were obtained using Cowan's codes [1] which show the need of comprehensive analysis of these spectra using high resolution data. New selenium high resolution emission spectra have been recorded on Fourier transform (FT) spectrometers at NIST covering the region 2400 Å to 1.5 µm and a 3m grating spectrometer at St. F. X. University covering wavelengths from 300 Å - 2400 Å. Sources for these spectra include high-current continuous hollow cathode (HCL) lamp and triggered spark discharges. The data for Se III in visible region were supplemented from the previously measured spectra by George [2] in the region of 360 Å– 1044 nm. The analysis led to the identification of about 1060 spectral lines in the wavelength region of (350Å – 1500nm) and the determination of 220 energy levels belonging to the Se I-III.

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Opacity Effect on Visible Neutral Helium Line Emissions and its Impact on Line Ratios

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Abstract:

In this work an effort has been made to investigate the intensities of neutral helium lines and their ratios taking into account the influence and consequences of opacity. For this purpose, helium escape factors have been calculated on the basis of some simplifying assumptions in the ADAS code, which is part of the well-known Atomic Data Analysis Structure (ADAS) database. The change in excited state population and ionization balance due to re-absorption of radiation is then derived using a collisional-radiative model based on calculations of the ADAS code. The opacity affected photon emissivity coefficients (PECs), basically effective rate coefficients, have been estimated for routinely detected visible neutral helium lines and their ratios have been derived for a specified plasma length and geometry of the system. It is found that the spectral lines 4921.9 Å ($2p^1P^o-4d^1D$) and 7281.3 Å ($2p^1P^o-3s^1S$) are slightly affected by opacity whereas the lines 4713.1 Å ($2p^3P^o-4s^3S$), 5047.7 Å ($2p^1P^o-4s^1S$) and 7065.7 Å ($2p^3P^o-3s^3S$) are strongly affected by opacity. Under opacity effects, the density sensitive helium line ratio He I 4921.9 Å/He I 5047.7 Å and temperature sensitive He I 7065.7 Å/He I 7281.3 Å can't be used accurately.

Reproducible Supercomputing for Laser-Plasma Modeling

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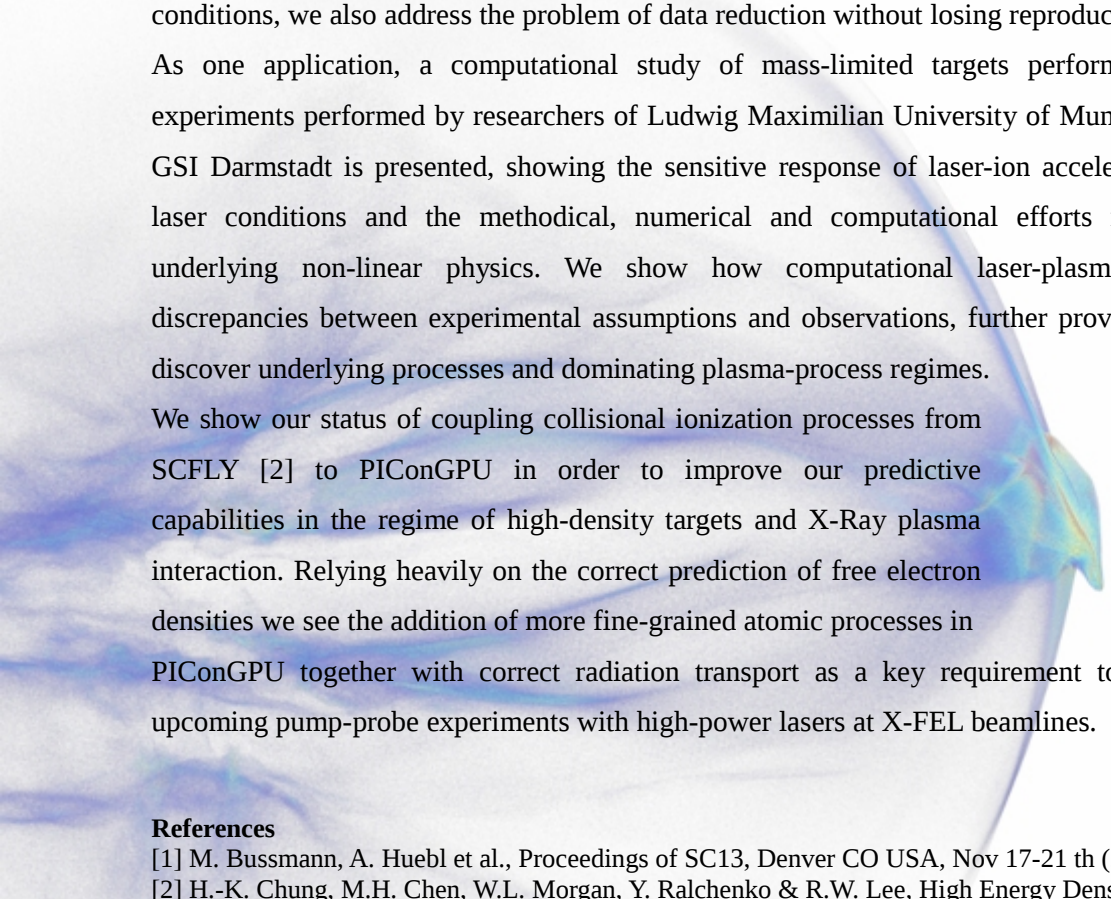
PICongPU is the worlds fastest particle-in-cell code due to its capability to run on modern, highly parallel compute hardware such as graphical processing units [1]. Not limited to, but driven by the demand for predictive capabilities in the domain of laser-plasma based, compact accelerators such as the laser-wakefield accelerator (electrons) and laser-ion acceleration, PICongPU is provided by the authors as an open-source code for the community to study the evolution of plasmas under extreme conditions with full dimensionality (3D3V).

Laser-matter interaction is determined by several fundamental processes that all interplay in today's experiments: the geometric evolution of electron and ion densities in full 3D, relativistic-mass increase and resulting relevance of the $\mathbf{v} \times \mathbf{B}$ term in Lorentz force in ultra-high fields, radiation damping and characteristic radiation signatures of electrons in high magnetic fields, ion-ion collisions in dense targets, field and collisional ionization processes and hard-photon induced processes by X-Ray beams in pump-probe setups, just to name a few. In order to provide predictive capabilities from theory and simulation modeling requires tremendous computational resources and even today creates easily PBytes of data per setup.

We present our approach using reproducible, scrutable, reviewed and testable algorithms implemented on supercomputers with modern hardware and modern computing models to enable numeric studies to investigate plasma physics. Striving for an improvement of our capabilities to add both a systematic error bar to the models used to describe laser-plasma interaction and a statistical error bar to its sensitivity to initial conditions, we also address the problem of data reduction without losing reproducibility.

As one application, a computational study of mass-limited targets performed in collaboration with experiments performed by researchers of Ludwig Maximilian University of Munich at the PHELIX laser at GSI Darmstadt is presented, showing the sensitive response of laser-ion acceleration on initial plasma & laser conditions and the methodical, numerical and computational efforts necessary to describe the underlying non-linear physics. We show how computational laser-plasma modeling can address discrepancies between experimental assumptions and observations, further providing in-situ diagnostics to discover underlying processes and dominating plasma-process regimes.

We show our status of coupling collisional ionization processes from SCFLY [2] to PICongPU in order to improve our predictive capabilities in the regime of high-density targets and X-Ray plasma interaction. Relying heavily on the correct prediction of free electron densities we see the addition of more fine-grained atomic processes in PICongPU together with correct radiation transport as a key requirement to describe and understand upcoming pump-probe experiments with high-power lasers at X-FEL beamlines.



femto-second scale proton
bunch created from a mass-
limited spherical target

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The effect of core-valence and core-core correlations on the energy levels and radiative transition probabilities along the Mg-like sequence

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This work is part of a general investigation which started two years ago in order to elucidate discrepancies between measured and theoretical line intensities. The key roles in the atomic calculations are played by the configurations included in the target representation along with the method describing the electron-impact collision strengths. We have theoretically investigated the accuracy of the energy levels and line intensity ratios [1] while performing the atomic-kinetics calculations via collisional radiative-model [2] of the experiment performed at the n-helix laser test bed facility at GSI [3]. Numerous intercombination and forbidden x-ray transitions belonging to the Li-like Al have been computed and a large part of them appeared blended in the measured spectrum along with some K alpha transitions belonging to Al V as given by our study. K alpha transitions have also been the subject of another one of our papers concerning the inner-shell photo-ionization x-ray lasing in C II [4] where extensive collisional-radiative modelling has been performed for both the laser-produced copper plasma that would generate the pumping radiation and the carbon lasing medium. The C II structure has been also computed within the R-matrix approach in another one of our papers [5] for providing consistency among the energy levels and radiative data with previous calculations.

It is worth mentioning that the accuracy of the energy levels and radiative transition probabilities is also affected by the inclusion of core-core and core-valence correlations in the configuration expansion. This can greatly influence the results in the case of iso-electronic series containing only a few electrons besides the closed-shell core. In a recent paper [6] we demonstrated that in the case of Mg-like S V the inclusion of additional 22 configuration state functions corresponding to electron promotion from the 2p subshell positively influenced both the energy levels and radiative transition rates. The calculations have been performed within the Flexible Atomic Code [7] framework. Here, another role is played by the selected fictitious mean configuration which significantly influenced the transition probabilities.

In this present work we are investigating the effect of core-core and core-valence correlations for the Mg-like iso-electronic sequence in order to explicitly see how this effect changes for different elements.

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Time-resolved XANES spectroscopy using a table-top laser-plasma source : study of copper under extreme conditions and out-of-equilibrium

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Out-of-equilibrium Warm Dense Matter

Ultrashort laser sources development enables nowadays the possibility for matter to reach both extreme density (\sim solid) and temperature ($\sim 10\,000$ K) conditions, or what we call “Warm Dense Matter”.

Neither plasma physics nor condensed matter models are able to give a good description of how matter behaves during this intermediate state. Lots of experimental and theoretical works are now in progress in this research field.

Moreover, working with femtosecond lasers leads to out-of-equilibrium phenomena during which a large amount of energy is deposited in the electrons while the lattice remains cold. Resulting thermal equilibration and phase transitions dynamics are still on the debate. A delayed fusion is predicted by quantum molecular dynamics simulations applied to noble metals (gold, silver, copper). This would be due to the stability reinforcement of the crystalline lattice, also known as “bond hardening” [1]. The latter is linked to the electronic d-band shift towards low energies, and has been invoked to interpret an electron diffraction experiment on a gold sample [2]. There is still a need for experimental evidence of this phenomenon.

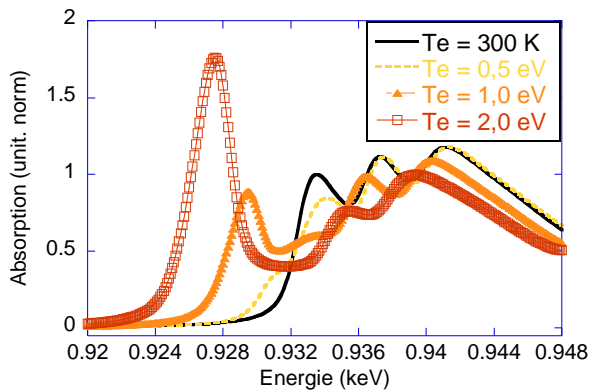


Fig. 1 : XANES spectra calculated near the copper L3-edge in out-of-equilibrium situations near solid density : cold lattice and different electronic temperatures.

Time-resolved XANES spectroscopy measurements on copper

XANES spectroscopy would be a way to experimentally highlight it. A study concerning the spectral range near the copper L3 edge (932 eV) using a synchrotron source has been recently published [3]. Electronic d-states are probed from $2p^{3/2}$ -states. A pre-edge is observed to be building up, which evolution gives the electronic temperature dynamics.

The shift of the electronic d-band during the out-of-equilibrium conditions may generate a spectral shift of this pre-edge (see Fig. 1), but hasn't been evidenced yet. We also think that the loss of the crystalline order should give rise to the disappearance of the post-edge structures.

Several experiments have been realized using Eclipse laser and a table-top station dedicated to time – resolved XANES measurements at CELIA laboratory [4]. At first, some XANES spectra have been acquired using a X-Ray source produced by the irradiation of a CsI solid target. This source duration of ~ 15 ps FWHM -approximately the equilibration thermal time of copper- restrained our temporal resolution. We used more recently a cluster Xenon jet to produce a X-Ray source of comparable emissivity but a significantly shorter duration (≤ 2.5 ps FWHM). Out-of-equilibrium XANES spectra have been registered and show the same pre-edge evolution as the one published by LNBL. Signal over noise ratio allows us to follow the evolution of the post-edge structure and deduce the associated dynamics of the loss of crystalline structure.

The observation of a spectral shift of the pre-edge and the validation (or not) of the « bond-hardening » requires an even shorter temporal resolution. This should be soon achieved by the mean of a betatron X-Ray source at LOA.

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Effective electron temperature measurement using Line intensity Ratio method in Ar-He multi ion species plasma

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Abstract

Optical Emission Spectroscopy is one of the non-invasive methods in determining electron temperature in plasmas. In this experimental work, we determine effective electron temperature in a filament discharge Argon-Helium multi ion species plasma under different working pressures between $5 \times 10^{-4} - 5 \times 10^{-3}$ mbar and discharge currents 0.4 – 1.2 A, using line intensity ratio method and single planar Langmuir probe. Both argon and helium schemes are used to determine the electron temperature and results are compared with Corona model. Langmuir probe results shows bi-maxwellian electron temperature at low neutral pressures and becomes single maxwellian at higher pressures. He neutral lines 728.1 nm ($3^1S - 2^1P$), 706.5 nm ($3^3S - 2^3P$) and Argon neutral lines 415.8 nm, 420.1 nm, 425.9 nm and ion lines 427.7 nm, 434.8 nm are used for line intensity ratio method.¹⁻³ Two different approaches have been applied for He line schemes and Argon line schemes. The excitation rate coefficient data for Helium lines is taken from ADAS database.

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Numerical and experimental study of magnetized accretion phenomena in young stars

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Newly formed stars accrete mass from the circumstellar disc via magnetized accretion funnels that connect the inner disc regions to the star. The ensuing impact of this free-falling plasma onto the stellar surface generates a strong shock, whose emission is used as a proxy to determine the accretion rates.

In general, the existence of a range of mass accretion rates and the presence of strong magnetic fields ($> \text{kG}$) on the stellar surface [1] entail a variety of behaviors for the post-shock plasma, with important repercussions on its dynamics, stability and detection. Observations show that the X-ray luminosity arising from the shock heated plasma at the base of accretion columns is largely below the value expected on the basis of optical/UV observations [2]. As a result, current 2D numerical simulations matching X-ray accretion rates cannot reproduce optical accretion rates [3].

To understand the impact of accretion flows on the stellar surface in the presence of a strong magnetic field we have developed laboratory experiments reproducing crucial aspects of the accretion dynamics in Young Stellar Objects. As a model of accretion columns, we use laser-produced super-Alfvénic magnetically confined jets [4,5] to collide them on solid targets. Here we present results from these experiments and from multi-dimensional MHD simulations.

Specific efforts are made to capture the fundamental differences between 2D and 3D simulations, in particular the existence of instabilities, the importance of radiation transport as well as the influence of plasma thermal/dynamic beta. We also present recent results aiming to control the time-variability of the laser-produced jets.

The authors acknowledge the support from the Ile-de-France DIM ACAV, from the LABEX Plas@par and from the ANR grant SILAMPA.

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Feasibility study of the direct electric field measurements in the RF sheath in front of the ICRF antennas

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Abstract

Ion Cyclotron Range of Frequencies (ICRF) heating is one of the auxiliary methods used to heat the plasma in the magnetic confinement fusion devices (tokamaks and stellarators). It is based on coupling the RF electromagnetic power into the core plasma. The RF electromagnetic waves are launched from an antenna located inside of the reactor vacuum chamber, close to the plasma boundary.

However, it is due to this proximity of the antenna to the plasma that the ICRF systems in the present day fusion machines are often experiencing spurious effects: sputtering, hot spots on the plasma-facing components and loss of coupling. The likely cause of these effects is the build-up of rectified electric potential in the RF sheath near the antenna. This potential, once combined with the static background magnetic field, accelerates the ions from the plasma towards the plasma-facing components thereby enhancing physical sputtering.

To address this issue, self-consistent computational models of the RF sheath and the edge plasma - antenna interactions are being developed. However, they lack direct experimental verification. One of the main parameters involved in the interactions is the electric field which should be measured in the antenna sheath.

The IShTAR (Ion Cyclotron Sheath Test Arrangement) device dedicated specifically to the investigation of the edge plasma-antenna interactions in the tokamak edge-like conditions, is used to develop the diagnostics for the electric field measurements for simplified antenna geometries required for the present-day RF sheath models. IShTAR is equipped with a helicon plasma source and a single strap ICRF antenna. It has simplified geometry and provides an easy access for the diagnostics.

IShTAR is used to develop and test a diagnostics for the electric field measurements based on the Stark effect modifying the optical emission spectrum in the presence of a DC electric field. A high-resolution spectrometer with an iCCD camera will observe through an optical fibre and collimating lenses the light emission originating from the RF sheath of the small region of the ICRF antenna. We present in this paper the first measurements in a Helium plasma and their comparison with one-dimensional analytical models of the Stark effect in a magnetised plasma.

Transport of intense photon pulses through dense helium gas at 60 – 65 eV

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Recently an experiment was performed at FERMI FEL, the purpose of which was to use short and intense light pulses to create a dense population of helium doubly excited states (DES) by means of a single photon absorption at ~ 60 eV in order to trigger self-amplified spontaneous emission. A strong emission line at 30.4 nm (40.8 eV) was detected in the perpendicular direction to the incoming beam.

Following the experiment we now study the transport of short (100 fs FWHM Gaussian) and intense (up to 10^{14} W/cm² peak power density) light pulses through a layer of dense helium gas (up to ≈ 1 mm length and 500 mbar pressure). The photon probe energy is varied in the $\omega_0 \sim 60 - 65$ eV region coinciding with the lowest lying DES of helium atoms. The physical process is simulated by the three-level lambda system governed by the Maxwell-Bloch equations where the upper state is one of the $n^+ 1P$ DES below the $N = 2$ ionization threshold. At the highest values of target pressure and probe intensity the simulations show that the resonantly tuned probe pulse is followed by noise-induced stimulated emission signal at $\omega \approx 40$ eV photon energy which saturates at distances comparable to the probe beam diameter ($\approx 50 \mu\text{m}$).

As theoretically predicted in 2003 [1], the energetically very close emission line could be observed in a three-body recombination Lyman- α laser on the $2p$ to $1s$ transition in He^+ ion at $\omega_R = 40.8$ eV. In this scheme, bare nuclei are the parent ions, which can be obtained by two-step photo-ionization, meaning that the pump energy has to be larger than 54.5 eV (the ionization energy of the ground state of the He^+ ion), which is true in the above mentioned experiment. The theoretical predictions indicate that considerable gain can be obtained for the Ly- α transition for gas densities as low as 10^{19} cm^{-3} and times of the order 100 – 200 fs, similar to life-times of doubly excited states.

The observed emission could therefore result from two conceptually different emission paths: stimulated resonant Raman scattering with direct emission from the doubly-excited states and stimulated XUV emission following three-body recombination to create inverted population of $\text{He}^+ 2p$ states in a fully ionized plasma. A good knowledge of atomic processes in plasma is indispensable to predict and explain the outcome of such experiments.

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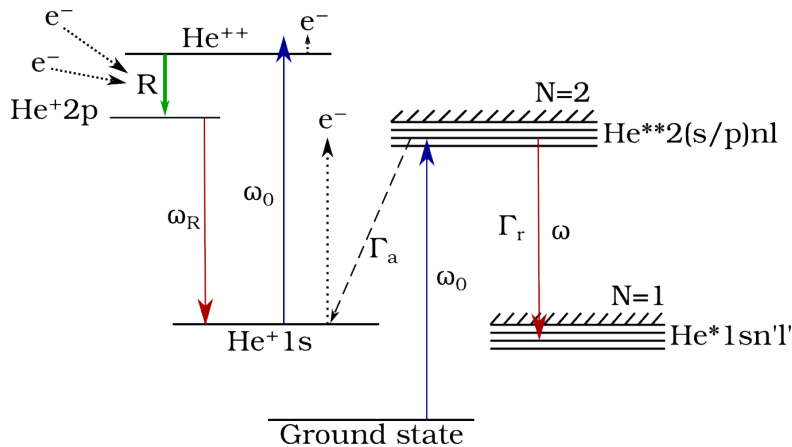


Figure 1: Schematic representation of two possible lasing schemes in helium.

***Electron impact ionization cross sections of
the ground and excited levels of Se^{3+}***

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Using a detailed level-to-level distorted-wave formalism, electron impact single ionization cross sections are theoretically investigated from the ionization threshold to 1000 eV for levels belonging to the ground and two lowest excited configurations of $[\text{Ni}]4s^24p$, $4s4p^2$, and $4s^24d$ of Se^{3+} . The detailed computation method can be found in work [1, 2]. The ionization cross sections of the two levels belonging to the configuration of $4s^24p$ are nearly equivalent and so are the $4s^24d$, whereas large difference is found for the eight levels belonging to the configuration of $4s4p^2$. The theoretical results are utilized to analyze and interpret a recent experimental measurement for the single-ionization cross section of Se^{3+} [3]. The population distributions existed in this experiment is diagnosed. Except for the levels of the ground configuration, there are also populations from levels of the excited configuration of $4s^24d$.

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Simplified yet accurate quantum theory on direct double ionization by a electron due to decoherence induced by Coulomb interaction

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Accurate quantum theory on electron-impact direct double ionization, which is commonly based on the atomic collision theory described by a fully correlated many-body Green function, poses unique challenges to theorists. It can, however, be simplified by proposing that the Coulomb interaction of the first ejected electron with a second one shifts the wave phases in an uncontrolled way and induces the loss of coherence. By fully taking advantage of the correlation features, simplified yet accurate quantum theory is formulated to investigate the energy correlations among the continuum electrons and energy resolved differential and integral cross section in the direct double processes according to the separation of knock-out (KO) and shake-off (SO) mechanisms. To demonstrate the effectiveness of our proposed approach, we apply it to investigate the electron impact direct double ionization of C^+ , N^+ , O^+ . The results show that the separate formulation offers an accurate description, which demonstrated the validity of the presumption of decoherence induced by the Coulomb interaction.

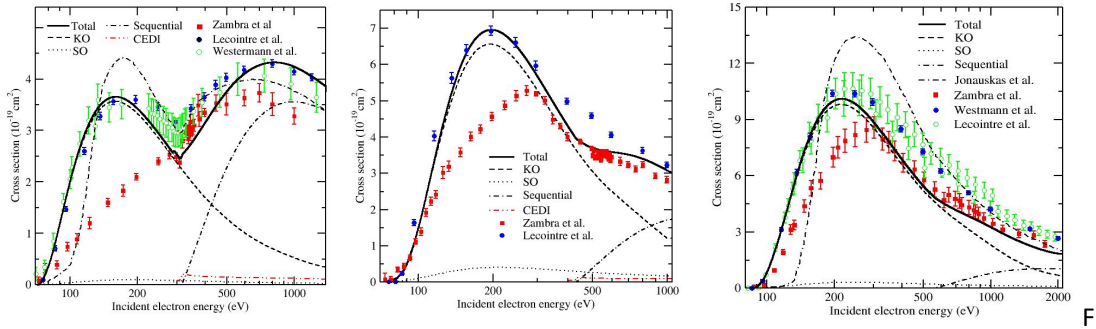


FIG. 1. Electron impact double ionization cross section of C^+ , N^+ and O^+ compared with experimental results by M. Zambra et al. [1] (red solid squares with error bars), M. Westermann et al. [2] and J. Lecointre et al. [3] (blue solid circles with error bars). Double ionization cross sections of knock-out, shake-off, and cascade mechanisms are displayed by red dotted line, green dashed line and blue dot-dashed line, respectively.

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Combination of discharge- and laser-produced plasmas for high brightness extreme ultraviolet (EUV) light sources

We present the concept of a compact EUV light source using a hybrid approach combining the techniques of discharge and laser produced plasmas. In this so called laser-heated discharge plasma (LHDP) approach a Z-pinch plasma is electrically generated and optically heated.

The goal of the project is to generate highly brilliant incoherent EUV radiation with minimum required laser pulse energy and discharge currents. To achieve this, the discharge of a triggered hollow cathode source produces and confines gas puff Z-pinch, which is used as a target for a pulsed CO₂ laser beam. The optical heating of the plasma will counteract radiation losses of the plasma pinch and thus prolong/increase the radiation of EUV emission [1]. Furthermore, any possibility for tailoring the emission spectra as well as the size of the emitting volume by focused laser radiation will be studied.

The general experiment was already set up within the group and performed successfully employing a 1064 nm Nd:YAG laser. The main absorption process of laser radiation inside the plasma is described by inverse electron-ion Bremsstrahlung which depends on a suitable combination of laser wavelength, plasma density and temperature. Due to a mismatch of achievable plasma density and fixed laser wavelength of 1064 nm, no significant effect was observed. A new setup utilizing transversely excited CO₂ lasers with 10.6 µm wavelength is currently build. The longer wavelength is expected to increase laser absorption within the plasma by a factor of up to 100.

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Investigation of radiation hydrodynamics properties in laser-produced silicon and tin plasmas

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A laser-produced plasma (LPP), formed by a high energy Q-switched laser pulse focused onto a solid target, consists of a large number of transient species and emits intense radiation from visible light to X-rays. The experimental observation and theoretical study of transient images and spectra of a LPP can reveal the energy level structures of atoms/ions, and carry rich information about the plasma structure and the related dynamic processes. In recent decades the LPP has gained universal acceptance as a standard laboratory ion source and pulsed short wavelength light source for important applications as light sources for extreme ultraviolet (EUV) lithography, EUV metrology and surface treatment and modification. LPP sources emitting soft X-rays in the water window are being developed for use in a number of novel microscope designs for water window imaging and cell tomography. For these applications optimization of conversion efficiency and/or brightness are the topics of major concern, while knowledge of ion distributions and velocities are essential in designing effective debris elimination schemes and evaluating the potential effects of ion impact on multilayer mirror surfaces.

Experimental device and theoretical model

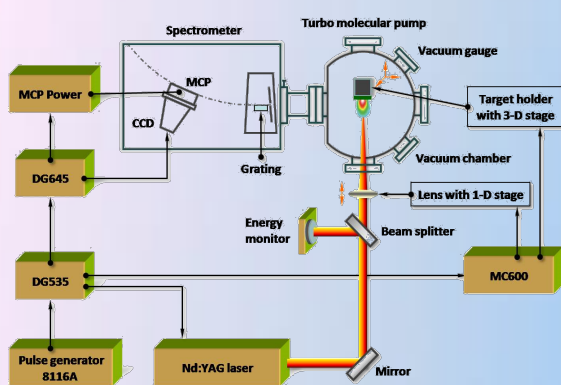


Figure 1 Schematic of the experimental setup used for laser produced plasma

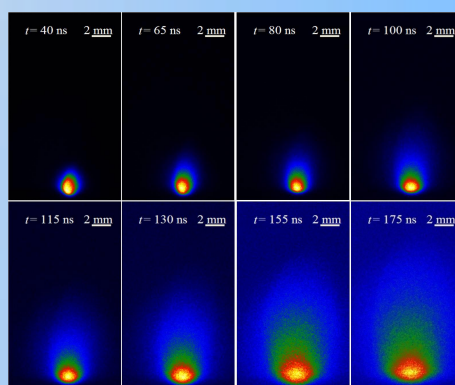


Figure 2 ICCD photographs of visible emission from laser-produced Si plume plasma at vacuum environment

we present a simplified radiation dynamic model based on the fluid dynamic equations and the radiative transfer equation. Meanwhile, calculation of the ionization balance and the charge states is respectively performed within the LTE model and the time-dependent collisional radiative model (CRM). By using the radiation dynamic model, the experimental spectra has been simulated, and furthermore the temporal and spatial evolution characteristics of the plasma temperature and density as well as the various transient particles have been investigated systematically.

The experimental and theoretical results of silicon plasma

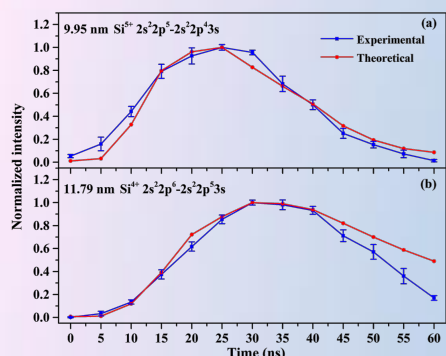


Figure 3 Normalized time-resolved spectral intensity of two peaks as a function of time delay

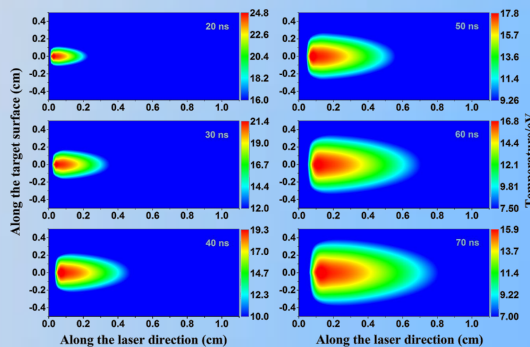


Figure 4 The temporal and spatial evolution of temperature in the silicon plasma

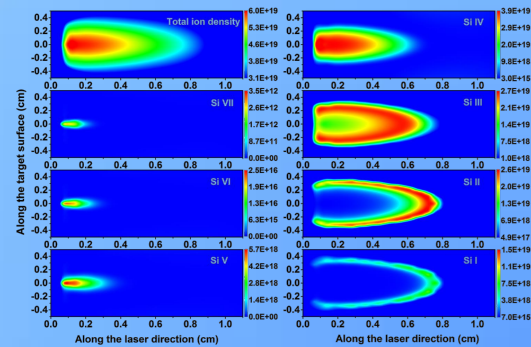


Figure 5 The distribution of different charge states in the silicon plasma at 70 ns time delay

The experimental and theoretical results of tin plasma

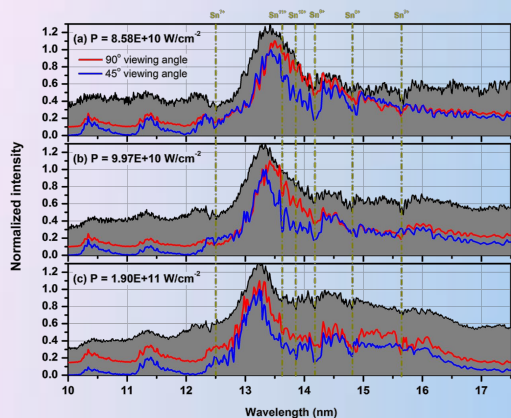


Figure 6 Normalized experimental and theoretical spectra of tin plasma with different laser power density

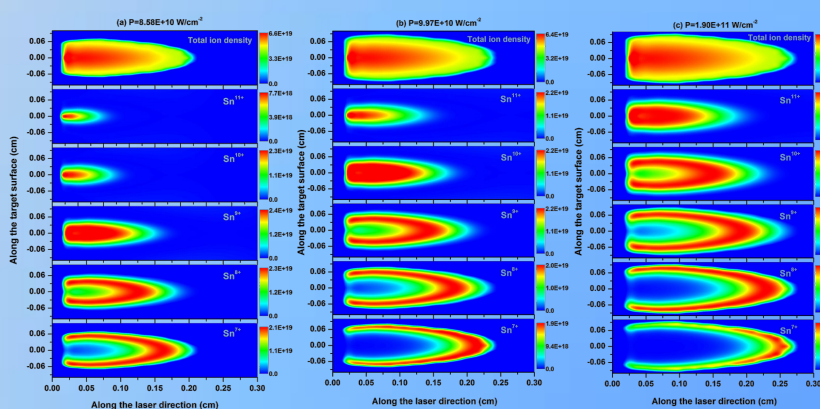


Figure 7 The distribution of different charge states in the tin plasma with different laser power density

Abstract

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Atomic data such as oscillator strengths and wavelengths are fundamental for astrophysical applications. With atomic data, one can derive abundances of specific elements in a star. Stars in the Galaxy keep the composition of the interstellar gas in which they were formed (Lambert, 1989; McWilliam, 1997; Nomoto et al. 2013), this in turn allows us to construct the evolution history of our Galaxy. Deriving abundances depends on several parameters together with atomic data, for this reason accurate and complete atomic data are essential. Inaccurate atomic data lead to uncertain abundances and prevent discrimination between different Galactic evolution models.

However, atomic data of some elements are incomplete or even missing, particularly for the infrared wavelength region. In our studies, we focus on the infrared region and neutral species that are present in cool stars. Magnesium is an important element to trace the α -element evolution in our Galaxy. In this study, we present a study of neutral magnesium, Mg I, with laboratory measurements together with atomic calculations to improve the atomic data of Mg I lines. We derived the oscillator strengths by combining the experimental branching fractions with radiative lifetimes reported in the literature or computed in this work. A hollow cathode discharge lamp was used to produce free atoms in the plasma and a Fourier transform spectrometer recorded the intensity-calibrated high-resolution spectra.

In addition to experimental work, we performed theoretical calculations using the multiconfiguration Hartree-Fock program, ATSP2K. We started with a calculation of the atomic state functions, $(\Psi(\gamma LS) = \sum_i c_i \Phi(\gamma_i LS))$.

These calculations were done in the simplest approximation where each ASFs consists of only one configuration state function, $\Phi(\gamma_i LS)$. In order to improve the ASFs, we systematically expanded CSFs which were formed from single and double replacements of orbitals in the reference configurations. Both the valence and the core valence correlations were accounted for.

Once the ASFs were determined, the oscillator strengths were calculated as expectation values of the transition operator. Our calculations include all the transitions from configurations with n up to 7 and l up to g , such as $3s2$, $3s3p$, $3s3d$, . . . $3s7g$. We performed calculations both in the length and the velocity gauges (Froese Fischer et al. (1997)). For the low lying terms, the agreement between the length and the velocity gauge oscillator strengths is as low as 5%, for the transitions involving the highest terms, this agreement gets slightly worse. We chose the velocity gauge as it weights more to the inner part of the wave function and shows good convergence properties which indicates more accurate oscillator strengths for transitions involving highest terms.

In addition, we examined the consequences of relativistic effects. We compared our results with results from Breit-Pauli approximations calculations where relativistic effects are accounted for. We found that the relativistic effects were negligibly small in our calculations except for the $1,3F_3$ terms. For the $4f\ 1,3F$ terms, we performed calculations with relativistic effects and applied the method of fine tuning (Brage & Hibbert 1989) to match with the experimental data.

This project provides a set of experimental and theoretical oscillator strengths. Overall, our theoretical lifetime values are in very good agreement with the previously published experimental values within 10% uncertainty. The theoretical oscillator strengths are in very good agreement with the experimental data and complement the missing transitions of the experimental data up to $n = 7$ from even and odd parity terms. This agreement makes us confident to recommend our theoretical values when the experimental data are not available or have high uncertainty.

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Calculation of Detailed Relativistic Electron Excitation Cross Sections and Application to Hydrogen-Caesium Plasma

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Electron impact excitation cross-sections and rate coefficients have been calculated using fully relativistic distorted wave theory [1] for several fine-structure transitions from the ground as well as excited states of caesium atom in the wide range of incident electron energy. These processes play dominant role in low pressure hydrogen-caesium plasma, which is relevant to the negative ion based neutral beam injectors for the ITER project [2]. As an application, the calculated detailed cross-sections are used to construct a reliable collisional radiative (CR) model [3] to characterize the hydrogen-caesium plasma. Other processes such as radiative population transfer, electron impact ionization and mutual neutralization of Cs^+ ion with negative hydrogen ion along with their reverse processes are also taken into account. The calculated cross-sections and the extracted plasma parameters from the present model are compared with the available experimental and theoretical results [4].

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Study of particle and impurity fluxes with the filter-camera system on Wendelstein 7-X stellarator

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Wendelstein 7-X stellarator is currently being prepared for the OP1.2 operation phase which is aimed for a first experiments with an island divertor configuration. One of the important diagnostic tools for a divertor region is the endoscope system, which consists of two sets of endoscopes. Once two endoscopes for each set are installed they will serve for a tomography of impurity distribution and measurements of 2D temperature and density profiles at the island divertor region. These measurements are important for a density control and impurity accumulation avoidance.

Each endoscope guides light to a detector box where a filter-camera system is located. The initial light beam is split into visible and ultraviolet. In order to record light a CCD cameras are used. In the case of ultraviolet light cameras are equipped with the image intensifier. To select emission lines of interest narrow band interference filters are used. All measurements are supported with an overview spectrometer. Five cameras for visible and ultraviolet range will simultaneously observe divertor with the same field of view [1].

For impurity transport studies, temperature and density determination five nozzles are located in the divertor target plane. One of the possibilities is to use thermal neutral helium injection to determine electron temperature and density. Such a technic was already used for the TEXTOR tokamak [2]. Corresponding collisional-radiative model which includes related physical processes, such as electron excitation and deexcitation, spontaneous emission and recombination processes, collision with heavy particles and other processes is needed. Moreover, related up-to-date cross sections are demanded.

When two endoscopes are available, it makes it possible two perform tomographic reconstruction of the 2D temperature and density profiles. During the operational phase OP 1.2a only one endoscope will be available and only line integrated results will be obtained.

A mock-up observation system with the filter-camera was built for the PSI-2 linear plasma device. Line integrated electron temperature and density profiles were obtained. Due to low values of these parameters available model gives poor agreement with the reference measurements made by a single Langmuir probe. Moreover, high reflectance of the inner part of plasma vessel also complicates the spatial reconstruction process.

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Strong higher-order resonant contributions to Fe K_{α} x-ray line polarization in anisotropic ~ 7 MK plasmas

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Resonantly captured electrons with energies below the excitation threshold are the strongest source of x-ray line formation in plasmas at $2 \leq T_e \leq 20$ MK containing highly charged Fe ions. The angular distribution and polarization of x rays emitted due to these processes were experimentally studied using an electron beam ion trap. Polarization due to dielectronic recombination of $Kr^{28+...34+}$ was measured using Compton polarimetry [1]. Later, the electron-ion collision energy was scanned over the KLL dielectronic, trielectronic and quadreelectronic recombination resonances of Fe and Kr ions with a resolution of ~ 6 eV [2]. The angular distribution of x rays was measured along and perpendicular to the electron beam propagation direction.

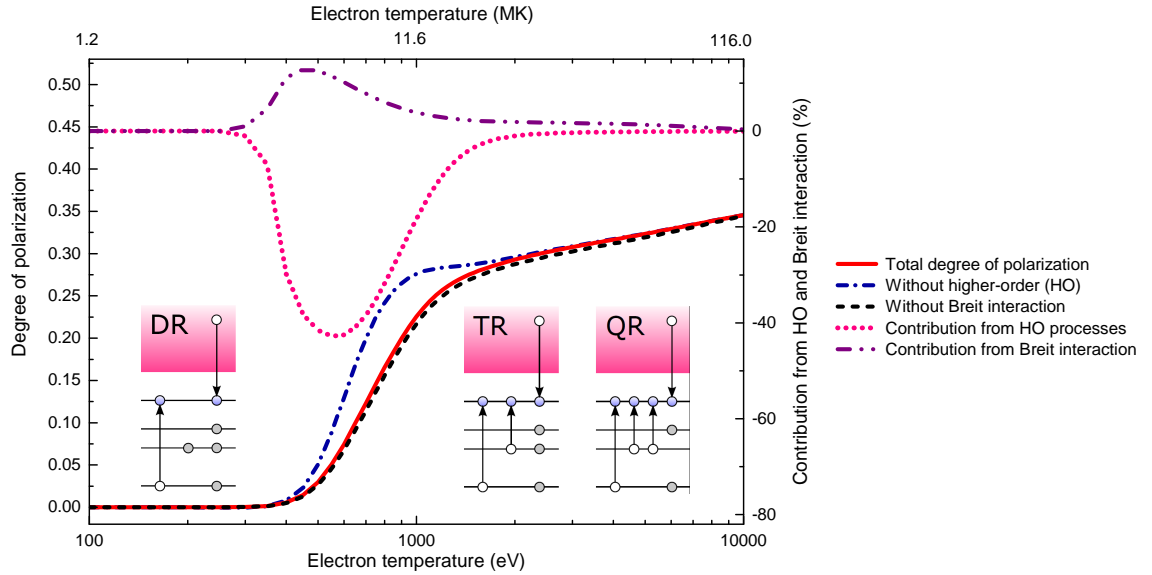


Fig. 1 Maximum polarization of iron K_{α} x rays due to resonant recombination as a function of the plasma temperature. Higher-order trielectronic and quadreelectronic recombination transitions dominate total polarization in the temperature range of 500–1500 eV (or 7–14 MK).

The data reveal the alignment of the populated excited states and show a high sensitivity of these parameters to the relativistic Breit interaction [1, 2]. We found that most of the transitions lead to polarization, including hitherto neglected trielectronic and quadreelectronic resonances. These channels dominate not only the ionization balance but also the polarization of the prominent K_{α} x rays emitted by hot anisotropic plasmas in a broad range temperature range (see Fig. 1). Our results comprehensively benchmark full-order atomic calculations done with the FAC [3] and RATIP [4] codes. We conclude that accurate polarization diagnostics of hot anisotropic plasmas, e. g., of solar flares and active galactic nuclei, and laboratory fusion plasmas of tokamaks can only be obtained under the premise of inclusion of relativistic and higher-order resonances which were neglected in previous work [2]. Furthermore, our experiments also demonstrates the suitability of resonant recombination angular distribution measurements for accurate directional diagnostics of electron or ion beams in the plasmas [5].

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Beam-Foil Plasma Creation during Ion-Solid Interactions

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Various atomic processes pertaining to basic plasma and astrophysical studies can be observed in typical interactions during the collisions between energetic projectile ions and target atoms. Study of these processes is very crucial to define the essence behind the underlying phenomena. In this connection, to explore the new insights of interactions, charge state evolution of energetic projectile ions (^{56}Fe , ^{58}Ni and ^{63}Cu) during the passage from thin carbon foils has been revisited in the 1.51-2.69 MeV/u energy range using the X-ray spectroscopy technique [1]. Advantageously, X-ray spectroscopy technique can measure the projectile charge state distribution (CSD) which is evolved only in the bulk of the foil unlike the electromagnetic techniques [2,3], which measure integrated CSD contributed from both the bulk and the exit surface of the foil. Interestingly, an unusual Lorentzian CSD is observed in contrast to the Gaussian distribution as found in the theoretical predictions [4,5] and the measurements using electromagnetic techniques [2,3]. The appearance of the Lorentzian charge state distribution is analogous to the CSD of ions in any plasma environment. The important aspect of this collisionally produced plasma, called beam-foil plasma is the high density and localized nature. The variation found between shapes of the observed and ETACHA [4] predicted CSDs may be attributed to the plasma coupling effects that are not considered yet in the theoretical codes and formalisms. Whereas, deviation from the experimentally measured CSD using the electromagnetic technique is due to the contribution from the multi-electron capture from the exit surface of the target [6]. It can be easily verified through the observed difference between the measured and calculated mean charge states in the present work and from the semi-empirical formalism [5], respectively. Thus, the charge changing processes leading to the CSD in the bulk of the solid, prominently influence due to the creation of localized plasma environment i.e. beam-foil plasma. Further, the laboratory high-density beam-foil plasma inheriting special properties can simulate the characteristics of the high-density plasma as seen in the stellar interior. Moreover, the creation of high-density plasma by the ion-solid interactions is found to be produced with intense heavy ion beams of the order of 10^{11} ions in 1 μsec pulse with high energy beams (~ 300 MeV/u) in GSI Darmstadt [7]. In contrast, we have observed that DC ion beam of low beam current ($\sim 10^{10}$ particles/sec) and intermediate energies (\sim few MeV/u) can also create such high-density plasma in solid targets. It will also be interesting to check the projectile energy ranges that can result in the beam-foil plasma.

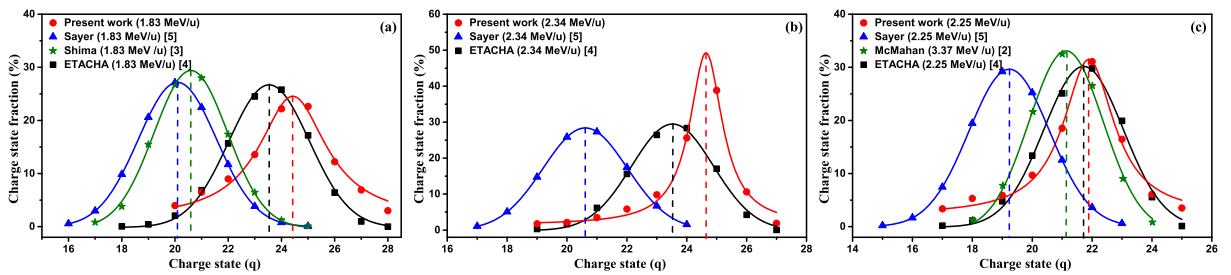


Figure 1: Comparison of the CSD and the mean charge states in the case of (a) ^{63}Cu (b) ^{58}Ni and (c) ^{56}Fe on ^{12}C for different beam energies. The figures show Lorentzian fit to the data of present work and Gaussian fit to all others. Errors are embedded in the symbols itself. The vertical dashed lines mark the mean charge states.

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“Soft x-ray spectroscopy of Dy, Er and Tm ions excited in laser-produced plasmas”

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Research involving the spectroscopy of highly charged lanthanide ions has gained momentum in recent years. The main driving force behind this resurgence owes in large part to the potential application of these ions in many high-profile fields, such as fusion, plasma diagnostics, soft x-ray lasers, next-generation lithography and water window source development [1 – 5]. The availability of high quality atomic data is crucial to the development of these fields. However, to date, very few spectroscopic studies of these ions have been undertaken. Furthermore, the complex structure of open 4f subshell ions makes accurate calculations of these spectra notoriously difficult. The aim of this study is to bridge the gap in our current understanding of soft x-ray radiation emitted from open 4d and 4f subshell heavy lanthanide ions.

Emission spectra of dysprosium, erbium and thulium ions created in laser-produced plasmas were recorded with a flat-field grazing incidence spectrometer in the wavelength range 2.5 – 8 nm. The ions were produced using a Nd:YAG laser of 7 ns pulse duration and the spectra were recorded at various power densities. The experimental spectra were interpreted with the aid of the Cowan suite of atomic structure codes [6] and the flexible atomic code (FAC) [7]. Above 5.5 nm the spectra are dominated by overlapping $\Delta n = 0$, $n = 4 - n = 4$ unresolved transition arrays (UTAs) from adjacent ion stages. The origin of an interesting feature located on the long wavelength side of these UTAs is examined. Following a detailed analysis, we have tentatively identified these features as $4d^2 \ ^3F_2 - 4d4f \ ^3G_3$ transitions in Sr – like ions. However, further experimental and theoretical validation is needed in order to clarify these assignments. Below 6 nm, $\Delta n = 1$, $n = 4 - n = 5$ transitions originating from ions with open 4d and 4f subshells give rise to a series of interesting overlapping spectral features. In addition, it was found that satellite transitions of the form $4f^{n-1}5s - 4f^{n-2}5s5g$ and $4d^{m-1}5s - 4d^{m-2}5s5p$ make a significant contribution to this region of the spectrum.

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EUV measurements of Y XXVII - Y XXXVII with an EBIT and magnetic dipole transitions suitable for plasma diagnostics

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Abstract:

Extreme-ultraviolet spectra of the L-shell ions of highly charged yttrium (Y^{26+} - Y^{36+}) were observed in the electron beam ion trap (EBIT) at the National Institute of Standards and Technology (NIST) using a flat-field grazing-incidence spectrometer in the wavelength range of about 4 nm to 20 nm. In order to reach the desired ionization stages, the beam energy was systematically varied from 2.3 keV to 6 keV during the experiment. The wavelength calibration was provided by the previously measured lines of neon, xenon, oxygen and iron. Fifty-nine spectral lines corresponding to $\Delta n = 0$ transitions within $n=2$ and $n=3$ have been identified using detailed collisional-radiative modeling of the non-Maxwellian EBIT plasma with uncertainties between 0.0003 nm and 0.0018 nm. Few of the identified lines were due to the forbidden magnetic dipole (M1) transitions within $2p^n$ configurations. To analyze the potential applicability of these lines to plasma diagnostics, large-scale collisional-radiative (CR) calculations were performed to generate Y spectra in Maxwellian plasmas with electron temperatures on the order of several keV; such high temperatures correspond to the maximal abundance of the L-shell ions of Y. It was found that several line ratios show strong dependence on electron density and/or electron temperature and hence may be implemented in diagnostics of hot plasmas, in particular, in fusion devices.

Electrical and Spectroscopic Investigations on Atmospheric Pressure Dielectric Barrier Discharge Plasma

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Abstract

The cold plasmas produced at atmospheric pressure are gaining major research focus due to their wide application range. Dielectric barrier discharges (DBD) are the most popular non-equilibrium glow-discharge or cold plasmas operated at atmospheric pressure. The dielectric barriers over electrodes are used to prevent glow-to-arc transition by limiting growth of discharge current. The glow discharge can be filamentary or uniformly diffused depending on the operating conditions. The electron energies in such plasmas may be substantially high to provide enhanced reaction rates. The important DBD applications include material processing, pollution control, plasma displays, UV lamps, plasma aerodynamics and plasma medicine etc.

Experiments have been performed to characterize a self-designed DBD plasma source operated at atmospheric pressure in helium gas. The dielectric-covered parallel-plate electrodes are energized with an AC high-voltage (2-5 kV) source of 1-20 kHz frequency. It is observed that the discharge remain stable & uniform in our parametric range. The discharge current & voltage waveforms were captured to justify the non-equilibrium nature of the discharge. Detailed spectroscopic measurements were performed to get plasma density and temperature through Helium-I line intensity ratio method. We have collected Helium line emissions from the glow discharge through visible spectrometer with attached CCD camera and analyzed the data for getting intensity. We have performed wavelength and absolute intensity calibrations required for my experiments. We have also obtained line intensities through computational code based on Collisional-Radiative (C-R) Model to estimate the electron plasma density and temperature. The electron density was obtained $\sim 1-2 \times 10^{11} \text{ cm}^{-3}$ while temperature was $\sim 3-8 \text{ eV}$ that are typical values for glow discharges. Further we have also found that selection of operating frequency and dielectric material are very crucial for getting discharge stability in DBD plasma.

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Spectroscopy of Sn highly charged ions

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Sn laser produced plasmas (LPPs) are of technological interest, being used as sources of extreme ultraviolet (EUV) light in nanolithographic applications. Due to the complex electronic configurations of the relevant ions $\text{Sn}^{7+...14+}$, arising from their open $4d$ subshell, spectroscopic investigation of these plasmas can be challenging. In particular, level and line identifications had been shown to be complex tasks [1,2]. We provide new spectral data and interpretation thereof, in both the optical and EUV regimes, obtained in a charge-state-resolved manner using an electron beam ion trap at the Max Planck Institute for Nuclear Physics in Heidelberg. Comparison with previous EUV measurements [1,2] indicates the need to re-evaluate identifications [3,4]. We also present the emission recorded on the ARC NL droplet-based Sn LPP source. These LPP spectra are difficult to interpret due to the intrinsic unresolved nature of the transitions and opacity effects arising from the high plasma density, but will provide detailed insight into the operation of a plasma source of EUV light.

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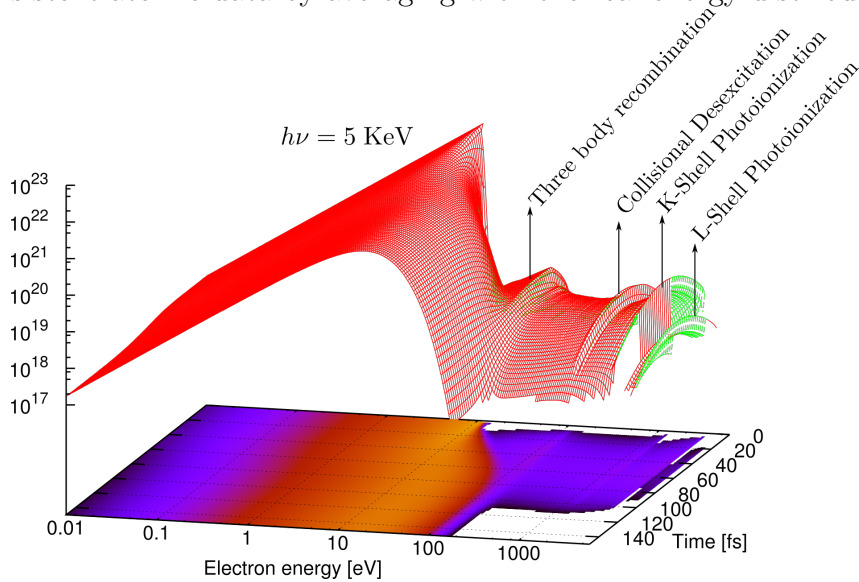
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Time dependent atomic physics in the interaction of X-Ray laser with matter

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The collisional radiative model is the most used method to study the ionization balance in plasmas out of equilibrium. To simulate the interaction of X-ray radiation with matter from ultrashort (20 fs) and ultraintense (10^{15} W/cm^2) X-ray laser, we use a non-local thermodynamic equilibrium (NLTE) collisional radiative model. Due to the strong non-equilibrium nature of the interaction of high energy photons with matter, it is not justified to assume a maxwellian or Fermi-Dirac distribution. Instead, it is necessary to include the thermal treatment of the distribution with the Fokker-Planck approximation. We consider additional inelastic collision processes with ions and source terms by interaction with the laser and other processes. This allows us to obtain more consistent atomic data by averaging with the real energy distribution.



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Collisional Quenching of Highly-Excited H₂ due to H₂ Collisions

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Collisional energy transfer involving H₂ molecules are of significant interest, since H₂ is the most abundant molecular species in the universe. However, accurate calculations of collisional energy transfer in the H₂ – H₂ system is still a challenging problem, especially for highly-excited H₂. Currently, most data are limited to initial rotational levels $j \leq 8$ or initial vibrational levels $v \leq 3$. The vast majority of these results involve some form of a reduced-dimensional approach which may be of questionable accuracy.

Currently, we are extending the $v=0$ data to higher j using the accurate potential energy surface (PES) for the H₂ – H₂ system developed by Patkowski *et al.* [1] and two quantum scattering programs (MOLSCAT [2] and vrrmm [3]). In order to solve the time-independent Schrodinger equation, the formalism for the scattering of two $^1\Sigma$ diatomic molecules described by Takayanagi [4] and Green [5], and the close-coupling(CC) formalism of Arthurs and Dalgarno [6] are employed. New inelastic quenching cross section for para-H₂+para-H₂ collisions with initial level $v = 0, j = 10, 12$ are shown in Figure 1.

Calculations for other de-excitation transitions from higher initial levels are still in progress. Collisions involving other types of hydrogen ortho-H₂+para-H₂, ortho-H₂+ortho-H₂ and para-H₂+ortho-H₂ will be considered in the future. Other future work involves vibrational transitions [7] with the full-dimensional PESs with full-dimensional scattering code TwoBC [8].

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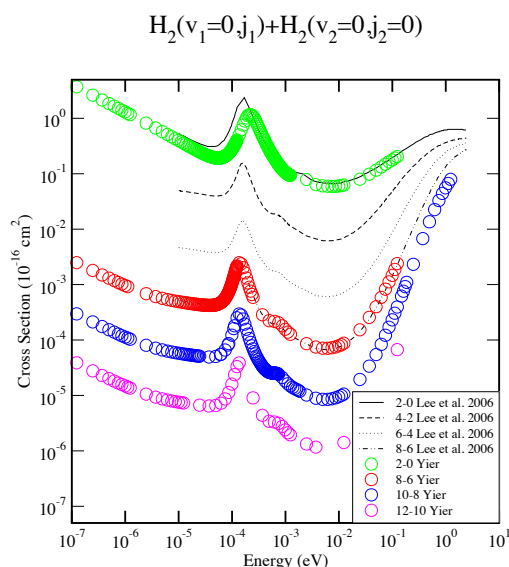


Figure 1: Cross section for the $v = 0, j$ level of H₂ in collisions with para-H₂ ($v = 0, j = 0$) as a function of the kinetic energy.

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Development of spectroscopy diagnostics for impurity transport study on Wendelstein 7-X

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The study of transport behavior of impurity ions in fusion plasma is a long-standing field of research. It's very important to prevent impurity accumulation in improved energy confinement regimes in order to maintain stationary plasma condition. The database in this field of impurity transport is by far not as large and detailed for stellarators as for tokamaks. Wendelstein 7-X (W7-X) is completed in October 2015, and currently the world's largest stellarator device. The divertor components will be ready before next operation phase (OP 1.2). Three major island divertor configurations with rotational transform values of 5/6, 5/5 and 5/4 have been designed to be used for edge exhaust. Measurement and analysis of edge impurity transport with different island configurations will lead to optimization of edge magnetic topology for steady-state operation.

The overview spectrometer is part of the endoscope system ^[1] which is being built by Forschungszentrum Jülich. The endoscope system contains 5 filter cameras (2 UV and 3 VIS filter camera), 1 IR camera and 5 spectrometers (2 UV, 1 VIS, 1 IR and 1 overview spectrometer). The main propose of this endoscope system is to measure electron density, electron temperature, impurity transport, hydrogen recycling and heat load in divertor region of W7-X. The overview spectrometer will be specified to monitor impurities contents at divertor region. It will be used for routine investigation of the impurity contents under different scenarios. It will also provide reference data for other diagnostics equipped on endoscope system, with which it share the same field of view.

Atomic data analysis methods are needed in order to extract information with physical meaning from rare data, such as spectral line shape fitting, excited level population density calculating, collisional-radiative modelling, and so on.

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Implementing atomic processes (ionization and collision) into particle-in-cell code to study proton stopping in partially ionization dense plasmas.

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A physical model based on a Monte-Carlo approach is proposed to calculate the ionization dynamics of dense plasmas within particle-in-cell simulations, and where the impact (collision) ionization (CI), electron-ion recombination (RE) and ionization potential depression (IPD) by surrounding plasmas are taken into consideration self-consistently. When compared with other models, which are applied in the literature for plasmas near thermal equilibrium, the temporal relaxation of ionization dynamics can also be simulated by the proposed model. Besides, this model is general and can be applied for both single elements and alloys with quite different compositions. The proposed model is implemented into a particle-in-cell (PIC) code, with (final) ionization equilibriums sustained by competitions between CI and its inverse process (i.e., RE). Comparisons between the full model and model without IPD or RE are performed. Our results indicate that for bulk aluminium at temperature of 1 to 1000 eV, i) the averaged ionization degree increases by including IPD; while ii) the averaged ionization degree is significantly over estimated when the RE is neglected. A direct comparison from the PIC code is made with the existing models for the dependence of averaged ionization degree on thermal equilibrium temperatures, and shows good agreements with that generated from Saha-Boltzmann model or/and FLYCHK code.

A Monte-Carlo approach to proton stopping in warm dense matter is implemented into an existing particle-in-cell code. This approach is based on multiple electron-electron, electron-ion and ion-ion binary collision and accounts for both, the free and bound electrons in the plasmas. This approach enables one to calculate the stopping of particles in a more natural manner than existing theoretical treatment. In the low-temperature limit, when “all” electrons are bound to the nucleus, the stopping power coincides with the predictions from the Bethe-Bloch formula and is consistent with the data from the NIST database. At higher temperatures, some of the bound electrons are ionized and this increases the stopping power in the plasmas as demonstrated by Zylstra et al. [Phys. Rev. Lett. 114, 215002 (2015)]. At even higher temperatures, the degree of ionization reaches a maximum and thus decrease the stopping power due to the suppression of collision frequency between projected proton beam and hot plasmas in the target.

Nuclear excitation with x-ray free-electron lasers - direct and plasma-mediated channels

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Long-lived nuclear excited states, also known as isomers, can store large amounts of energy over long periods of time. The study of such isomers could give new insights into nuclear structure, and also could initiate a number of fascinating potential applications related to the controlled release of nuclear energy on demand, e.g., novel energy storage solutions. Especially advantageous for the latter could be the $^{93\text{m}}\text{Mo}$ isomer, since an energy of 2.4 MeV can be freed by investing only 4.8 keV for the nuclear excitation to an above lying triggering level subsequently decaying to the ground state. Here, we study this so-called isomer triggering by considering the direct and secondary nuclear excitation by an x-ray free electron laser interacting with a solid-state nuclear target.

When driven at the resonance energy, the x-ray free electron laser can produce direct photoexcitation. However, in this laser-target interaction, the dominant process is the photoelectric effect producing a cold and very dense plasma. In such a plasma, secondary processes such as nuclear excitation by electron capture may also occur [1]. We develop a realistic theoretical model to quantify the magnitude of the secondary excitation taking into account the temporal plasma dynamics after the laser pulse [2]. Numerical results show that depending on the nuclear transition energy and the temperature and charge states reached in the plasma, secondary nuclear excitation by electron capture may dominate the direct photoexcitation by several orders of magnitude, as it is the case for the 4.8 keV transition from the isomeric state of ^{93}Mo , or it can be negligible, as it is the case for the 14.4 keV Mössbauer transition in ^{57}Fe . These findings are most relevant for future nuclear experiments at x-ray free electron laser facilities

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Collision data for molecular hydrogen plasmas

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The accurate modelling of low temperature plasmas that contain molecules requires state resolved molecular data to compute partition functions, opacities and emissivities. Although for both electron- and photon-molecule data there is a lack of comprehensive state-resolved data ($i, v_i, J_i \rightarrow f, v_f, J_f$) available, particularly for transitions that involve electronically excited states. In addition, for electron-molecule scattering convergence studies are rarely performed and hence there is a lack of accurate theoretical collision data for the major scattering processes.

At Los Alamos National Laboratory (LANL) and Curtin University we have embarked on the project of calculating *ab-initio* electron- and photon-molecule data for industrial and astrophysically relevant diatomic molecules. Combining these data with the suite of atomic, equation of state and plasma codes at LANL, we plan to model LTE (and possibly non-LTE) plasmas under a range of conditions and calculate opacities.

Recently we applied the *ab initio* convergent close-coupling (CCC) method to electron scattering from the hydrogen molecule H_2 [1] and its hot (vibrationally excited) ion H_2^+ [2]. Convergence of the major scattering processes has been explicitly demonstrated in the fixed-nuclei approximation. For H_2^+ cross sections were obtained for each vibrational state of the molecule. Adiabatic-nuclei calculations of H_2 are currently in progress and electronic, vibrational and rotationally resolved data will be obtained.

In the first step of the *ab-initio* photon-molecule project we have performed semi-adiabatic (includes coupling electronic-nuclei angular terms) calculations of state-resolved photo-dissociation of H_2^+ . Results are in excellent agreement with Babb [3] for the $2p\sigma_u$ state (who did not present $2p\pi_u$ photo-dissociation results). We found that the radiative dissociation cross section via the $2p\pi_u$ state is several orders of magnitude larger than the $2p\sigma_u$ photo-dissociation cross section for photon-wavelengths between the 40-100 nm range. As far as we are aware, radiative dissociation or association via the $2p\pi_u$ and higher excited states have not been accounted for in the rate coefficients, abundances, partition functions and opacities utilized in astrophysical models.

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