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The Calculation of Satellite Line Structures in Highly Stripped Plasmas

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Abstract

This is the final report of a three-year, Laboratory Directed Research and Development (LDRD) project at the Los Alamos National Laboratory (LANL). Recently developed high-resolution x-ray spectrographs have made it possible to measure satellite structures from various plasma sources with great detail. These lines are weak optically thin lines caused by the decay of dielectronic states and generally accompany the resonance lines of H-like and He-like ions. The Los Alamos atomic physics and kinetics codes provide a unique capability for calculating the position and intensities of such lines. These programs have been used to interpret such highly resolved spectral measurements from pulsed power devices and laser produced plasmas. Some of these experiments were performed at the LANL Bright Source and Trident laser facilities. The satellite structures are compared with calculations to diagnose temperatures and densities. The effect of non-thermal electron distributions of electrons on calculated spectra was also considered. Collaborations with Russian scientists have added tremendous value to this research due to their vast experience in x-ray spectroscopy.

Background and Research Objectives

Satellite lines are produced in hot plasmas by the radiative decay of an autoionizing level into a 1s vacancy. Autoionizing levels are generally populated by inner shell excitation, inner shell ionization, and dielectronic capture. Since satellite lines are generally excited-to-excited transitions, they are optically thin, and in principle should provide excellent diagnostics of density and temperature, because the radiation is unperturbed by the surrounding plasma. However, these lines are weak compared to resonance lines, and they have very complicated structures. Spectrographs of very high resolution are required to separate structures into component lines, and very accurate calculations are necessary to identify individual lines. Such spectrographs with high resolution in the range of 2-10 angstroms have been developed at the Multi-charged Ion Spectra Data Center (MISDC), in

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Moscow, Russia, which is a division of the Russian equivalent of the National Institute of Standards and Technology. MISDC is involved in high-resolution spectroscopy experiments at installations throughout the world.

Independently, a suite of atomic physics and kinetic codes have been developed at LANL.¹⁻² The atomic physics codes can be used to calculate a data base that can be used for plasma modeling. The Cowan ATomic Structure (CATS) code is an adaptation of the atomic structure codes of R.D.Cowan. The input to CATS consists of an the element, its stage of ionization, and a list of electron configurations. CATS solves the Hartree-Fock equations with relativistic corrections for each orbital of each input configuration. Fine structure levels are generated for each configuration and intermediate coupling and configuration interaction are included using perturbation theory. Energy levels and their designations, wavefunctions, Slater integrals, mixing coefficients, and oscillator strengths for transitions between levels are stored on the atomic data files. Plane-wave Born (PWB) electron impact excitation cross sections may also be optionally calculated. The Another Collisional Excitation (ACE) code is used to provide higher quality electron impact cross sections than those calculated by CATS. The distorted wave method with CATS atomic structure is used to calculate the improved cross sections. The General Ionization Program for Processes involving Electrons and Radiation (GIPPER) code uses CATS atomic structure to compute cross sections for ionization processes. The processes considered include photoionization, electron impact collisional ionization, and autoionization. Various methods of calculation are available and distorted wave continuum functions are employed. CATS, ACE, and GIPPER can operate in both configuration average or detailed fine structure mode. These codes write files for the database in a consistent format.

The Fine Structure Non-Equilibrium (FINE) code is used for modeling non-equilibrium plasmas. The necessary data is read directly from the atomic physics files discussed above. FINE can perform kinetics calculations based on fine structure, configuration average, or composite state models. Rate coefficients for collisional ionization, photoionization, autoionization, collision excitation, and radiative excitation are calculated directly from calculated cross sections, while the inverse processes three-body recombination, radiative recombination, dielectronic capture, collisional deexcitation, and radiative decay are calculated using the principle of detailed balance. Rate coefficients can be calculated using arbitrary electron distributions and radiation fields. The population models include local thermodynamic equilibrium, coronal equilibrium, collisional-radiative, steady-state, quasi-steady state, time-dependent, and effective schemes. FINE can produce various types of spectra based on the calculated populations and with different choices of line shapes and widths.

A preliminary collaboration between MISDC and Los Alamos revealed that the Los Alamos atomic physics codes produce results of sufficient accuracy to identify individual lines in these very complex structures. In particular, previously unregistered lines in beryllium-like magnesium observed in laser-plasma experiments were assigned initial and final state designations with help from the LANL codes. Several papers were published based on the results. It was the early success of this work that motivated the LDRD project.

The availability of various types of data was another motivation for this project. MISDC has access, through collaborations, to a wealth of high-resolution experimental data, especially for laser produced plasmas. In addition, MISDC collaborates with the Lebedev Physical Institute in Moscow and Cornell University. Plasmas produced by X and Z pinch experiments at these laboratories are studied using high-resolution spectroscopy. The satellite structure of the elements from Mg and Cu are being studied using both laser produced plasmas and X and Z pinch plasmas. The studies should provide insight to the important processes involved in each type of plasma. For instance, laser experiments with superdense plasmas (between the critical and solid densities) are of particular interest for comparisons with the Z and X pinch experiments.

The project also has provided the opportunity to study the effect of nonequilibrium electron distributions. The pinch experiments can produce plasmas with electron densities near 10^{23} and currents between electrodes can produce 5-15 keV electron-beam-like conditions passing through the resulting plasma. This situation is similar to the hot non-thermal electrons produced by the interaction of long wavelength (e.g. carbon dioxide lasers) and short pulse high intensity lasers with plasmas. Even though the existence of the hot electrons are well known, they are ignored in modeling calculations and it is standard procedure to use equilibrium electron energy distributions. Thus, for more accurate modeling of these plasmas, distributions with some representation of the hot nonthermal electrons are required. The LANL codes have been well suited for such calculations because the raw collisional cross-sections are used in the codes, instead of rate coefficients where the distribution is built in.

The project has also provided the opportunity for LANL experimenters to gain experience with the high-resolution MISDC spectrograph at local facilities. MISDC personnel have visited Los Alamos for several years to perform experiments at the LANL Bright Source and Trident laser installations. The visits have produced many interesting spectra that have resulted in several publications. It has been beneficial for LANL scientists to share experience and knowledge with the Russian collaborators.

Another motivation for this project was superior computing facilities at LANL. Fast computers with large memories were required to perform modeling and simulations

necessary to confirm the experimental results. Thousands of atomic energy levels were used in some of the calculations to obtain spectroscopic accuracy. The Russian collaborators did not have access to any comparable facility.

Importance to LANL's Science and Technology Base and National R&D Needs

The use of high-resolution spectrographs for detecting satellite lines has the potential for becoming a powerful diagnostic for various plasmas encountered in LANL research. The technique could be used as a diagnostic for nuclear weapons technology, inertial confinement fusion research, the National Ignition Facility, and for plasmas produced by pulsed power devices. In addition, the spectroscopic signature produced by hot electrons could prove useful for understanding nonthermal effects in plasmas. Developing models to calculate the intensities of these complex line structures is a formidable challenge to the LANL competency area of computer modeling and simulation.

This work provides a basic understanding of the principal processes, which populate autoionizing states for different types of plasma producing devices. The satellite structures for the same element in different devices can be studied. Each device will produce different plasma conditions that will change the satellite structure. The observations will provide a systematic procedure for developing plasma diagnostics. In addition, these structures will be studied as a function of atomic number, and possibly determine elements with the best diagnostic properties.

This work also provides an understanding of the effects of nonthermal electron distributions on the spectral properties of satellite structures. These effects are important and not well understood. For example, these electrons will change the spectral profile due to the increased importance of inner shell excitation and ionization. Effective electron energy distributions will be determined which characterize the experimental spectra. Diagnostics that are sensitive and/or insensitive to the nonthermal electrons have been determined. This aspect is related to collaborative research and development agreements involving digital displays, lighting systems, and other plasma processing devices involving electron beams or nonthermal electrons. In addition, hot electrons are very important for the fast igniter scheme proposed for inertial confinement fusion.

Scientific Approach and Accomplishments

The basic experimental technique employed involves using the Focusing Spectrograph With Spatial Resolution (FSSR-1D) spectrograph to observe the x-rays emitted from the plasma source under consideration. The FSSR-1D spectrograph utilizes a spherically bent mica crystal and the basic apparatus is described elsewhere³.

The theoretical technique to accomplish the goals of the project involves two steps. For the first step, the atomic physics codes CATS, ACE, and GIPPER are used to calculate a data base of cross sections for the appropriately chosen configurations of the ion stages for the element under consideration. The calculated data includes energy levels, oscillator strengths, electron impact excitation cross sections, electron impact ionization cross sections, photoionization cross sections and autoionization rates. The second step involves using the FINE code to access the previously calculated data base and compute the level populations for the appropriate plasma environment. The calculated populations are then used to simulate spectra. FINE is usually run by varying the plasma conditions until agreement with the experimental measurement is obtained. The major accomplishments of this project are outlined below.

Silicon. The Los Alamos Bright Source Laser, a high intensity subpicosecond laser, was used to produce a silicon plasma. This XeCl laser had a 400 fs pulse duration with a flux density of $4 \times 10^{18} \text{ W/cm}^2$. The high-resolution, high-luminosity FSSR-1D spectrograph was used to record the spectrum. The satellites to the Lyman- α Si XIV resonance line, caused by $2p3l - 1s3l$ radiative transitions were observed for the first time. The wavelengths of these lines were measured with a relative accuracy of 0.0008Å and an absolute accuracy of 0.0015Å. For improvement in the absolute accuracy measurement the uncertainties in the wavelengths of the reference lines must be reduced. This can be done in the future both experimentally and theoretically by using modern quantum electrodynamics ab initio methods for wavelength calculations of the reference lines $2p^2 \text{ } ^1D_2 - 1s2p \text{ } ^1P_1$ and $2s2p \text{ } ^1P_1 - 1s2s \text{ } ^1S_0$. In addition, we found the average plasma temperature to be 460 eV and density to be approximately $6 \times 10^{22} \text{ cm}^{-3}$. The small value of electron temperature and the large value of electron density (greater than critical density for $\lambda=308 \text{ nm}$) indicate that the x-ray plasma emission occurs mostly in the spatial region between the critical point and the solid surface in our experiment. Figure 1 (top) shows the experimental spectra, Figure 1 (bottom) shows the spectrum calculated by FINE. Note the good agreement between experiment and theory for both line positions and relative intensity, in particular, even for such subtle details as the three weak blue lines to the right of the large resonance line.

Aluminum. Spectroscopic measurements of an aluminum plasma produced by the XP pulsed power generator at Cornell University was recorded and studied. A high-resolution spectrograph using a spherically bent mica crystal was employed. Satellite lines from the Li-like to C-like ion stages of aluminum were observed in the direction of the

anode. Such lines appeared weakly or were absent in the direction of the cathode. The occurrence of these satellite lines is attributed to the formation of an electron beam caused by inductance of hot spot electrons to the anode. These highly energetic electrons collide with relatively cold ions causing K-shell vacancies, which leads to the observed satellite x-ray emissions. A collisional-radiative model based on a non-Maxwellian distribution of electrons was used to study the observed satellite structures. The electron distribution consisted of a thermal part to represent the plasma electrons and a Gaussian part to represent the electron beam. The study shows that these structures can be reproduced by calculations with electron beam fractions $f \sim 10^{-7}$, in agreement with experimental estimates. The calculations also suggest that a temperature gradient from approximately 30 to 80 eV is formed in the plasma. In addition, various aspects of the spectral properties of the plasma due to temperature and electron beam strength were studied. Figure 2 (left) shows a comparison between experiment and theory for the radiation produced by the Be-like ion stage. Figure 2 (right) also shows how the spectra changes as a function of beam fraction.

Magnesium. The role of hot electrons on the observed spectrum of three different laser produced magnesium plasmas was studied. The experiments, in part, were carried out at the Los Alamos Trident laser facility. In each case, the model calculations are compared to high-resolution spectroscopic measurements. The hot electrons, which provide enhanced direct collisional excitation, play a role in all three experiments and are essential for interpreting the 600 fs Nd-glass and the carbon dioxide laser spectra. The effect of hot electrons on the 1 ns Nd-glass spectrum is less pronounced, as expected. Calculations show that the presence of hot electrons can alter the spectroscopic interpretation of electron density derived from standard thermal methods. Hot electrons can intensify the intercombination line relative to Li-like satellites creating the appearance of a less dense plasma. In addition, hot electrons can also create a Li-like spectra, which appears to be produced by a much denser plasma. Estimates for the electron density, electron temperature, and hot electron fraction attained in each experiment are given. The spectra produced by the 600 fs laser pulse can be interpreted as being produced by a relatively cold plasma near the target surface interacting with hot electrons accelerated from the critical surface toward the target. Figure 3 show a comparison of theory and experiment for the 600 fs case, which is strongly dependent on hot electrons. More quantitative determinations of the electron energy spectrum are necessary.

Spectral measurements of magnesium plasma using the laser at the Max-Born Institute were studied. Many spectral lines and their associated wavelengths in the Be and

Li like ion stages were identified for the first time. The spectral observations were used to extract the plasma conditions.

Origination of Blue Satellites. A new mechanism for the origination of blue satellites in dense plasmas has been proposed. The mechanism is based on the collisional transfer of population between autoionizing levels. Atomic structure calculations show that the proposed mechanism holds for a wide class of ions, Be to Mo, due to the exact incorporation of the (n, L, S, J) split level structure. A complete analysis of the redistribution effects between the autoionizing levels of He_α and He_β show valuable density diagnostic properties for typical conditions of fusion plasmas, and the required spectral range is extremely small. Our analysis should serve as a benchmark for future theoretical and experimental investigations.

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Figure 1. Intensity (arbitrary units) as a function of wavelength (angstroms). The top figure corresponds to the silicon spectra recorded at the Bright Source laser facility and the bottom figure corresponds the calculation by FINE at a temperature of 460 eV and a electron density of 6×10^{22} .

Figure 2. The figure on the left is a comparison of the measured intensity (arbitrary units) from the Cornell X-pinch experiment with theory as a function of wavelength (angstroms). The wavelength range presented corresponds to emission from the Be-like ion stage. The solid curve is experiment and the dashed curve is theory corresponding to $N_e=1 \times 10^{19}$, $kT=60$ eV, and a hot electron fraction of 10^{-7} . The figure on the right corresponds to the calculated spectrum for different fractions of hot electrons as indicated at $N_e=1 \times 10^{19}$, $kT=60$ eV.

Figure 3. A comparison of the measured intensity (arbitrary units) from the 600 fs Trident laser shot with theory as a function of wavelength (angstroms). The solid curve is experiment and the dashed curve is theory. The parameters $N_e=5 \times 10^{21}$, $kT=180$ eV, and a hot electron fraction of 0.1 were used in the calculation.