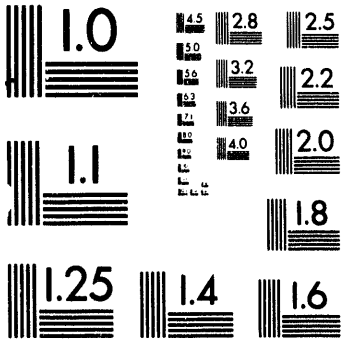
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PROGRESS REPORT FOR 1992-1993 ON

THE INVESTIGATION OF ELECTRON-ION RADIATIVE AND DIELECTRONIC RECOMBINATION IN HIGH-TEMPERATURE PLASMAS

Verne L. Jacobs (Principal Investigator)
Condensed Matter and Radiation Sciences Division,
Code 6693
Naval Research Laboratory
Washington, D. C., 20375-5345

(202) 404-7147

Prepared For

Dr. Michael D. Crisp
Fusion Theory Branch
Advanced Physics And Technology Division
Office of Fusion Energy
Office of Energy Research
Department of Energy
Washington, D. C. 20585

MASTER

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PROGRESS REPORT

I. Unified Description of Radiative and Dielectronic Recombination

A density-operator approach to the unified description of radiative and dielectronic recombination of atomic ions in high-temperature plasmas has been developed. Our objective has been the self-consistent incorporation of the effects of charged-particle collisions and plasma electric fields. This density-operator approach provides the desired generalization of our previously developed unified description, which gives corrections to the conventional independent-processes approximation in a low-density plasma environment. A noteworthy aspect of new generalization is the use of Liouville-space (tetradic) projection-operator techniques to provide a comprehensive framework for the incorporation of collisional and radiative relaxation processes. A manuscript, entitled "Influence of Relaxation Phenomena in the Unified Description of Resonant and Non-Resonant Radiative Transitions", by V. L. Jacobs, J. Cooper, and S. L. Haan, is nearly ready for submission to the Physical review A. This manuscript is devoted primarily to the comprehensive presentation of the general theory. The detailed expressions for the unified density-dependent electron-ion photo-recombination cross sections will be presented in a second manuscript, which is in preparation. It should be emphasized that this generalization of our low-density unified theory provides a self-consistent description of relaxation phenomena for a diverse class of atomic radiative transitions involving autoionizing resonances.

II. Calculations for Specific Dielectronic Satellite Transitions

Specific calculations are in progress for K-shell dielectronic satellite transitions in the He-like and Li-like ions of Fe and Ar, using the autoionization and radiative transition rates that have been provided by M. Chen, at the Lawrence Livermore National Laboratory. These rates were obtained from fully-relativistic multi-configuration atomic-structure calculations and are expected to be the most precise rates that are available. The main emphasis in these calculations is directed at spectroscopically resolvable dielectronic recombination satellites, which are produced by transitions involving relatively low values of the captured-electron principal quantum number. These resolvable features are expected to be the most sensitive to the corrections that are due to the use of a unified theory. The density-independent unified corrections to the independent-processes cross section have been provided by our previously-published theory, while the generalization under development will provide the additional corrections that depend on the plasma density. Comparisons will be made between the predictions of the low-density independent-processes theory, the low-density unified theory, the density-dependent independent-processes theory, and the density-dependent unified theory. The Ar satellite spectra is of particular interest for diagnostic studies on the MIT Tokamak, and a collaboration on the modeling of the relevant spectra has been discussed with E. Marmar, at the MIT Plasma Fusion Center. The Fe satellite spectra has been the subject of extensive experimental investigations at the Princeton Plasma Physics Laboratory, and a collaboration with members of the PPPL group on the simulation of the Fe K_α satellite spectra has been published, as described in detail in the following paragraph.

III. Modeling of K_α Dielectronic Satellite Spectra

The K_α model for the dielectronic satellite spectra of highly-charged Fe ions, which we have developed based on the conventional independent-processes theory of dielectronic satellite line intensities, has been incorporated into the muti-ion-species transport code MIST, which has been developed at the Princeton Plasma Physics Laboratory. This transport-simulation project has been carried out in collaboration with M. Bitter of PPPL and P. Beiersdorfer of LLNL. Excellent agreement has been obtained between the simulated spectra and the observed Fe K_α spectra from PLT and TFTR. A manuscript on this work, entitled "High-Resolution Measurements, Line Identifications, and Spectral Modeling of K_α Transitions in Fe XVIII - Fe XXV", by P. Beiersdorfer, T. Phillips, V. L. Jacobs, K. W. Hill, M. Bitter, S. Von Goeler, and S. M. Kahn, has been published in the Astrophysical Journal, Vol. **409**, 846, 1993. We have concluded that these satellite spectra can be employed to provide a very detailed investigation on the nature of the various plasma transport processes, both collisional and anomalous. Future extensions of this collaboration may be focused on the intimate coupling between the impurity-ion transport and radiative cooling problems, which we believe to be an important aspect in the realistic investigation of atomic processes in Tokamak plasmas. In addition, consideration is being given to an extension of the present atomic physics model to include contributions from the higher-lying autoionizing configurations with an electron in an n=3 quantum level. It may also be desirable to develop a new atomic physics model for the analogous dielectronic satellite spectra of Kr. A Kr satellite model would be useful for the study of plasma transport processes on the ITER Tokamak, where the electron temperature is expected to enter the region from 10 to 20 KeV.

IV. Effects of Electron Collisions and Electric Fields

A detailed investigation has been completed on the dielectronic recombination satellite spectra in the presence of a distribution of plasma electric microfields, taking into account both radiationless electron capture and inner-shell electron excitation as mechanisms for the population of the autoionizing states. A manuscript has been published in the Physical Review **A 44**, 1281, 1991, entitled "Effects of Electric Microfields on Argon Dielectronic Satellite Spectra in Laser-Produced Plasmas", by L. A. Woltz, V. L. Jacobs, C. F. Hooper, Jr., and R. C. Mancini. This investigation utilizes the conventional independent-processes theory of dielectronic satellite intensities, but it is based on a self-consistent treatment of the level-population and line broadening phenomena associated with autoionization processes, radiative transitions, electron collisions, and the quasi-static action of the ion-produced electric microfields. The calculations have been carried out for the lowest-lying n = 2 satellites, which are affected by the electric fields only in high-density laser-produced plasmas (with $N_e \sim 10^{24}$ cm^{-3}). For application to the lower-density conditions in Tokamak plasmas (with $N_e \sim 10^{14}$ cm^{-3}), a number of alternatives are under investigation for determining the dielectronic recombination rates associated with the Rydberg autoionizing states corresponding to large values of n. This collaborative investigation has resulted in the development of a model for the effects of electric fields which is more detailed than the original description presented in 1976 by V. L. Jacobs. We have now made substantial progress in the further extension of this investigation to incorporate an explicit calculation for the population densities of the n = 2 autoionizing levels as functions of the strength of the electric microfield. Detailed calculation will also be carried out for the enlarged manifold consisting of the n=2 and n = 3 states, using the fully-relativistic multi-configuration autoionization and radiative decay rates supplied by M. H. Chen, at LLNL.

V. Density-Sensitive Dielectronic Satellite Lines

A manuscript entitled "Observation of Density-Enhanced Dielectronic Satellite Spectra Produced During Subpicosecond Laser-Matter Interactions", by A. Zigler, V. L. Jacobs, D. A. Newman, P. G. Burkhalter, D. J. Nagel, T. S. Luk, A. McPherson, K Boyer, and C. K. Rhodes, has been published in the Phys. Rev. **A 45**, 1569, 1992. This work provides a convincing experimental verification of the earlier theoretical predictions, which were published in Phys. Rev. **A 21**, 525, 1980, by V. L. Jacobs and M. Blaha, on the density sensitivity of certain prominent dielectronic satellite lines in dense plasmas. The subject of this investigation has also been restricted to the n = 2 autoionizing levels, which produce the spectroscopically resolvable satellite features. However, the experimental confirmation of the theoretically-predicted density enhancement of the dielectronic satellite spectra has important implications for the realistic modeling of the dielectronic recombination rates associated with the higher values of n, which are affected by collisional processes at lower densities. It should be emphasized that the higher-n autoionizing levels usually provide the dominant contributions to the recombination rates of low- and medium-Z ions for plasma electron densities in the Tokamak regime.

VI. Polarization of Atomic Radiative Emission in Crossed Electric and Magnetic Fields

Motivated by the existence of the Lorentz electric field in Tokamak plasmas, which is perpendicular to the magnetic field, an investigation has been initiated on the angular distribution and polarization of atomic radiative emission in the presence of crossed electric and magnetic fields. Our previous work on the circular polarization of radiative emission in the presence of a magnetic field, which was reported in Phys. Rev. **A 36**, 3267, 1987, by V. L. Jacobs and J F. Seely, was carried out in relation to a proposed spectroscopic method for the determination of the poloidal magnetic field in a Tokamak plasma. Density-operator techniques provide the most natural means of accomplishing the objectives of the more general investigation of polarized atomic radiative emission, which has been given particular urgency as a result of new contacts with two different experimental programs. The first program is being carried out at the Sandia National Laboratories on the PBFA II device, where broad spectroscopic features have been observed in the presence of strong crossed E and B fields. The second program is in progress at the Harvard-Smithsonian Center for Astrophysics and involves the investigation of the effects of an electric field on dielectronic recombination rates. An additional application for this general density-operator analysis could be the more precise interpretation of the X-ray emission spectra of highly-charged ions which have been obtained from the EBIT device at the Lawrence Livermore National Laboratory.

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VII. PROGRESS

A unified expression for the total photo-recombination cross section has been derived, for one autoionizing state and single-electron plus single-photon continua[20] but allowing for degenerate magnetic sublevels and multiple partial-wave contributions in the partial-wave expansion for the electron-continuum state. For the simple case in which the angular-momentum degeneracy and the partial-wave expansion are not taken into account, we recover the unified result of Alber, Cooper, and Rau[18]. We have recently extended the unified description to multiple electron- and/or photon- continua, using a projection operator approach[38], and we will include degeneracy and the partial-wave expansion.

The conventional expression for the dielectronic recombination rates has been evaluated to obtain predictions[26] for the K_α satellite spectra due to the ions Fe XVIII-Fe XXIV in the characteristic density and temperature region of Tokamak plasmas. Account has been taken of all fine-structure components of the $2p \rightarrow 1s$ radiative transitions from autoionizing states populated by both dielectronic recombination and inner-shell-electron collisional excitation.

The effects of indirect processes involving autoionization resonances have been investigated for electron-density sensitive line-intensity ratios, and the resonance contributions have been found to be comparable with the direct electron-impact excitation rates for magnetic-quadrupole transitions in highly-charged ions. A manuscript will be submitted to the Physical Review A, in collaboration with P. L. Hagelstein, M. H. Chen, and J. F. Seely.

VIII. PROPOSED INVESTIGATION

Using a projection-operator approach, the unified description of radiative and dielectronic recombination will be extended to treat processes involving more than a single state of the initial ion, the autoionizing resonance, and the recombined ion, including specifications of angular-momentum quantum numbers.

The investigation of the K_α dielectronic satellite spectra for highly-charged iron ions will be extended to include n=3 autoionizing levels and to evaluate the interference contributions to the satellite line intensities. Using the PPPL impurity-ion transport code, a realistic simulation of the observed Fe K_α spectra will be produced for comparison with the PLT and TFTR X-ray observations[25]. Particular attention will be given to transport-sensitive lines.

A density-matrix description will be developed in order to extend the unified description of radiative and dielectronic recombination to self-consistently incorporate the effects of charged-particle collisions and plasma electric microfield distributions. Specific calculations will be carried out for K-shell dielectronic satellite transitions in Fe and Ar ions of interest for the diagnosis of Tokamak plasma, using both the conventional and the unified theories for the spectral line shapes.

IX. COORDINATION WITH CURRENT TOKAMAK OBSERVATIONS AND ELECTRON-ION BEAM MEASUREMENTS

The high-resolution Fe X-ray spectra[25] that has been obtained from PLT and TFTR offer a unique opportunity for a comparison between Tokamak observations and theoretically-predicted dielectronic satellite spectra. In order to make a realistic comparison, it will be necessary to take into account radiative emissions by ions moving in and out of different temperature and density regions, using the PPPL impurity-ion transport code. Of particular interest will be the effects on the K_α satellite spectra due to departures from the standard corona equilibrium model, in which impurity ion transport is neglected and the ionization and recombination processes are assumed to be in a static balance. If the ionization and recombination rates could be predicted with sufficient confidence, it should be possible to deduce information on the precise nature of the ion transport mechanisms from transport-sensitive satellite lines.

The electron-ion beam experiments at JILA[11] and ORNL[12], which have confirmed the theoretically-predicted[9] electric-field induced enhancement, may provide sufficient resolution of the dielectronic recombination cross sections to enable a more precise comparison to be made between the results of the unified and conventional theories. The Livermore Electron Beam Ion Trap (EBIT), which has been successfully employed to observe the dielectronic satellite spectra of highly-charged ions[39], is expected to provide experimental spectra that could be compared with the results of precise calculations.

X. RELATED WORK ON RADIATIVE EMISSION PROCESSES IN CRYSTALS

A theoretical investigation of radiative emission by energetic electron beams propagating through crystals has been in progress in the Condensed Matter and Radiation Sciences Division. Recently, this investigation has been directed at the treatment of free-bound and bound-bound transitions[40], which are in many ways analogous to the atomic radiative and dielectronic recombination processes under study in this investigation. In the crystal radiation processes, the electron beam is directed nearly along an axis or plane of the crystal symmetry. Electrons from the beam may be captured into states which are bound in the transverse direction, giving rise to the coherent process of channeling radiation. It appears that the resonance-scattering, projection-operator, and density-matrix approaches, which we are developing for the unified treatment of radiative and dielectronic recombination, could also be employed for a unified treatment of the analogous radiative emission processes in crystal lattices. An important aspect in our description of radiation processes is the self-consistent treatment of the excited-level populations and spectral-line shapes, taking into account the same set of elementary autoionization, collision, and radiation processes.

XI. COLLABORATIONS

This investigation is being accomplished by means of collaborations with the following exceptionally-qualified atomic theorists:

Professor J. Cooper, University of Colorado, is collaborating in the development of the unified description of radiative and dielectronic recombination and in the incorporation of charged-particle collisions and plasma electric-fields into this description, using a density-matrix approach.

Professor S.L. Haan, Calvin College, is also collaborating in the development of the unified description of radiative and dielectronic recombination, particularly in the generalization of this description to allow for multiple autoionization and radiative-decay channels.

Dr. Manfred Bitter, Princeton Plasma Physics Laboratory, and Dr. Peter Beiersdorfer, Lawrence Livermore National Laboratory, are collaborating in the simulation of the Fe K_α satellite spectra for comparison with the PLT and the TFTR X-ray observations[25].

Dr. M.H. Chen, Lawrence Livermore National Laboratory, will be able to generate fully-relativistic multi-configuration results for autoionization and radiative decay rates, together with photoionization cross-sections, as required for the precise evaluation of the unified expressions for the intensities of individual dielectronic satellite transitions.

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XIV. RESUME

Verne Louis Jacobs	1964 B.S.	Massachusetts Institute of Technology (Physics)
Research Physicist		
Complex Systems Theory Branch	1968 Ph.D.	University of California at Berkeley (Physics)
Condensed Matter and		
Radiation Sciences Division		
Naval Research Laboratory		

Dr. Jacobs has carried out research work on a wide variety of topics in the fundamental quantum-mechanical theory of atomic autoionization, collision, and radiation processes, and he has incorporated new theoretical descriptions of these processes into the prediction of the charge-state distributions and the radiative emission spectra of atomic ions in high-temperature laboratory and astrophysical plasmas. His Ph.D. thesis research was an investigation of electron-electron correlation effects on the energy-level structure and radiative properties of K- and L-shell atoms. During his research associate appointments at the Weizmann Institute of Science (1968-71), at the Queen's University of Belfast (1971-72), and at the NASA Goddard Space Flight Center (1972-74), he carried out extensive theoretical and computational investigations of forbidden radiative transitions, multiple-photon processes, and photoionization processes in two-electron atoms, with particular emphasis on processes involving the autoionzing states that are relevant to dielectronic recombination.

In 1974, Dr. Jacobs joined Science Applications Inc. and worked (under contract for the Naval Research Laboratory) on the calculation of dielectronic recombination rates and on the modeling of the ionization structure and the radiative emission spectra of high-temperature laboratory and astrophysical plasmas. After joining the Naval Research Laboratory in 1977, he completed investigations on the effects of plasma electric microfields on high-Rydberg autoionizing states and on the effects of angular-momentum-changing electron collisions on dielectronic satellite spectra. He has also developed a comprehensive and systematic description for the multiple ionization and X-ray radiation produced by inner-shell-electron ionization processes and for the broadening of spectral lines by autoionization, collision, and radiation processes. Dr. Jacobs has made internationally recognized contributions to the fundamental quantum-mechanical theory of atomic photoionization, photoelectron angular distributions, multiple-photon and forbidden radiative transitions, inner-shell-electron processes, and dielectronic recombination. He has maintained extensive collaborations with leading atomic physicists at Universities and Government Laboratories on both the fundamental quantum-electrodynamical theory of atomic processes and the theoretical prediction of spectral-line intensities from the high-temperature plasmas encountered in fusion research and laser-matter interaction studies. In 1985, Dr. Jacobs was elected to Fellowship in the American Physical Society.

XV. PUBLICATION LIST

Verne Louis Jacobs

Research Physicist

Code 4694

Condensed Matter And Radiation Sciences Division

Naval Research Laboratory

Washington, D. C. 20375-5000

(202) 404 7147

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