DOE/ER/14134--8

DOE/ER/14134-08

ELECTRON COLLISIONS WITH POSITIVE IONS

FINAL REPORT

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June 15, 1990 - June 14, 1992

May 1997

Prepared for the U.S. Department of Energy under Contract No.
DE-FG05-90 ER 14134

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This report concerns a program of computation of cross sections for electron impact excitation and ionization of ions. This is the final report which covers the period from June 15, 1990 to June 14, 1992 for grant No. DOE-FG05-90ER14134.

A review /1/ of progress made in the 1980s for calculations on electron impact excitation of atoms and ions for low and intermediate energy ranges concludes that the effect of continuum channels is very important to include in close coupling calculations. This may be achieved by use of pseudostates or the coupled-channels optical-potential method or the intermediate energy R-matrix method. Those methods have been applied mainly to electron atom scattering to date and much remains to be accomplished in electron-ion scattering. Further, for multicharged ions, contributions of excitation-autoionization and resonant-excitation-double-autoionization to total ionization cross sections are important and underscore the role of two-electron correlation effects. Electron excitation data for alkali-like ions are reviewed in /2/.

Detailed calculations are given for excitation-autoionization and resonant-excitation-double-autoionization contributions to electron impact ionization cross sections for Li-like ions in /3/. Twelve autoionizing states arising from the $1s2s^2$, $1s2s2p$, $1s2p^2$, $1s2s3s$, and $1s2s3p$ configurations, together with the ground $1s^22s$ and excited $1s^22p$, $1s^23s$, $1s^23p$, and $1s^23d$ states, are included in a close-coupling expansion. The cross sections are calculated at a large number of energy points and are then convoluted with a 2.0eV full-width-at-half-maximum Gaussian to simulate an experimental energy spread. Various measured features by Hofmann et al. /4/ are reproduced well by the calculations.

Electron excitation cross sections are reported /5/ for the $3s^2S \rightarrow 3p^2P$ resonance transition in Mg^+ at energies from threshold to approximately nine times threshold (40 eV). Experiments are performed using electron-energy-loss and merged-beams methods. Calculations are made in two five state close coupling approximations. In addition, fifteen-state close coupling calculations made in /6/ are used to determine the forward-to-backward correction required to extract experimental cross sections for $4s^2S \rightarrow 4p^2P$ in Zn^+ .

Relative level populations and density-sensitive emission-line ratios $R_1 = I(18.687 \text{ nm})/I(19.351 \text{ nm})$, $R_2 = I(19.664 \text{ nm})/I(19.351 \text{ nm})$, and $R_3 = I(19.105 \text{ nm})/I(19.351 \text{ nm})$ were derived /7/ using calculations /8,9/ of electron impact excitation rates for Fe XII. Excellent agreement was found with observations of solar active region and flare spectra obtained by the Naval Research Laboratory's S082A slitless spectrograph on board Skylab. The electron densities deduced from the Fe XII line ratios are also in agreement with those determined from Fe XIII and Fe XIV.

During the contract years 1990-92, Dr. Henry spent 20% of his time working on this contract. Dr. Tayal spent 100% of his time.

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- DOE/ER/14134-01 Fe XII line ratios in solar flares.
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- DOE/ER/14134-06 Close-Coupling Calculations for the Electron-Impact Excitation of Zn^+
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- DOE/ER/14134-07 Excitation cross sections for the $ns^2S \rightarrow np^2P$ resonance transitions in Mg^+ ($n=3$) and Zn^+ ($n=4$) using electron-energy-loss and merged-beams methods
S.J.Smith, A.Chutjian, J.Mitroy, S.S.Tayal, R.J.W.Henry, F.-F. Man,
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Reports:

- DOE/ER/14134-03 Electron Collisions with Positive Ions: Progress Report: 6/90 - 6/91
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- DOE/ER/14134-08 Electron Collisions with Positive Ions: Final Report: 6/90 - 6/92.
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