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ELECTRON-IMPACT IONIZATION OF HEAVY ATOMIC IONS

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ABSTRACT

General theoretical methods for the calculation of direct and indirect processes in the electron-impact ionization of heavy atomic ions are reviewed. Cross section results for Xe^{8+} and U^{89+} are presented.

Electron-impact ionization cross sections for heavy atomic ions are important for the modeling of high temperature plasmas found in controlled fusion[1] and x-ray laser research[2]. For heavy atomic ions in low stages of ionization, indirect processes may make substantial contributions to the electron ionization cross section. Contributions to the single ionization cross section can be made by the following processes,

$$e^- + A^{q+} \rightarrow A^{(q+1)+} + e^- + e^- , \qquad (1)$$

and

$$e^- + A^{q+} \rightarrow [A^{q+}]^* + e^- \quad \hookrightarrow A^{(q+1)+} + e^- , \qquad (2)$$

where A represents an arbitrary ion with charge q. The first process is called direct ionization and the second is called excitation-autoionization. The inner-shell excited atomic ion, denoted by $[A^{q+}]^*$, may also radiatively stabilize,

$$[A^{q+}]^* \rightarrow A^{q+} + h\nu , \qquad (3)$$

and thus not contribute to ionization. For heavy atomic ions in moderate to high stages of ionization, the radiative decay channel becomes quite important. Contributions to the double ionization cross section can be made by the following processes,

$$e^- + A^{q+} \rightarrow A^{(q+2)+} + e^- + e^- + e^- , \qquad (4)$$

and

$$e^- + A^{q+} \rightarrow [A^{(q+1)+}]^* + e^- + e^- \quad \hookrightarrow A^{(q+2)+} + e^- . \qquad (2)$$

The first process is called direct double ionization and the second is called ionization-autoionization.

For most electron ionization calculations we have used the atomic structure codes developed by R.D. Cowan.[3] Bound state energies and wavefunctions are generated in either the standard Hartree-Fock (HF) approximation or the Hartree-Fock approximation with relativistic modifications (HFR), which includes the mass-velocity and Darwin terms within modified differential equations.[4] Intermediate-coupled eigenvalues and eigenvectors are obtained by diagonalization of a Hamiltonian matrix which contains both configuration-interaction and spin-orbit integrals. For certain electron ionization calculations we have used the atomic wavefunction code developed by I.P. Grant.[5] Bound state energies and wavefunctions are generated in the standard Dirac-Fock (DF) approximation.

A non-relativistic or semi-relativistic direct ionization cross section is calculated in a configuration-average distorted-wave approximation.[6] The target ion is described by a HF or HFR approximation and the partial waves ($k\ell$) are computed in HF or HFR frozen-core potentials. A fully relativistic direct ionization cross section is calculated in a sub-configuration-average distorted-wave approximation.[7] The target ion is described by a DF approximation and the partial waves ($\varepsilon\ell j$) are computed in DF frozen-core potentials. General purpose computer codes have been written based on the configuration-average ionization cross section (CAION) and the sub-configuration-average ionization cross section (SCAION).

A non-relativistic or semi-relativistic excitation-autoionization contribution to the total ionization cross section is calculated in either of two computational schemes. In the first scheme[8] a configuration-average distorted-wave excitation cross section is statistically partitioned over all levels of the final excited configuration. The indirect contribution to the total cross section is then summed taking explicit account of both the energy position and branching ratio of each excited level calculated using Cowan's atomic structure codes. If the atomic structure calculations show that certain excited levels are bound, their contribution to the total cross section is of course ignored. The configuration-average method works well when most of the levels within the final excited configuration are above the ionization limit, the branching ratios for autoionization are all close to one, and correlation in the initial and final states is small. In the second scheme[9] a distorted-wave excitation cross section is calculated for each and every level of the final excited configuration. The indirect contribution to the total cross section is then summed in the same manner as the configuration-average method. The level to level method is able to handle those cases where only a few levels within the final excited configuration are above the ionization limit and where branching ratios for autoionization are not close to one. In addition, configuration-interaction effects are easily incorporated into a level to level method. A suite of general purpose computer codes have been written based on the configuration-average and level to level methods for obtaining excitation-autoionization contributions to the total ionization cross section.

A study[10] of the electron-impact ionization of Xe^{8+} provides a good example of the various ionization processes discussed in the first paragraph. In Fig. 1 experimental crossed-beams measurements are compared with configuration-average distorted-wave calculations for single ionization from the $4d^{10}$ ground configuration of Xe^{8+}. The dashed curve is the sum of direct ionization cross sections for the 4d, 4p, and 4s subshells. The largest excitation-autoionization contributions to the total ionization cross section come from the transitions $4p \to 4f$, $4p \to 5d$, $4p \to 5f$, $4p \to 6p$, $4s \to 4f$ and $4s \to 5s$. Since the observed threshold for ionization is between 112 eV and 121 eV, in contrast to the $4d^{10}$ ground configuration calculated value of 182.2 eV, and the theoretical results are substantially below the measurements at the cross section peak, we suspect that the ion beam has a metastable component.

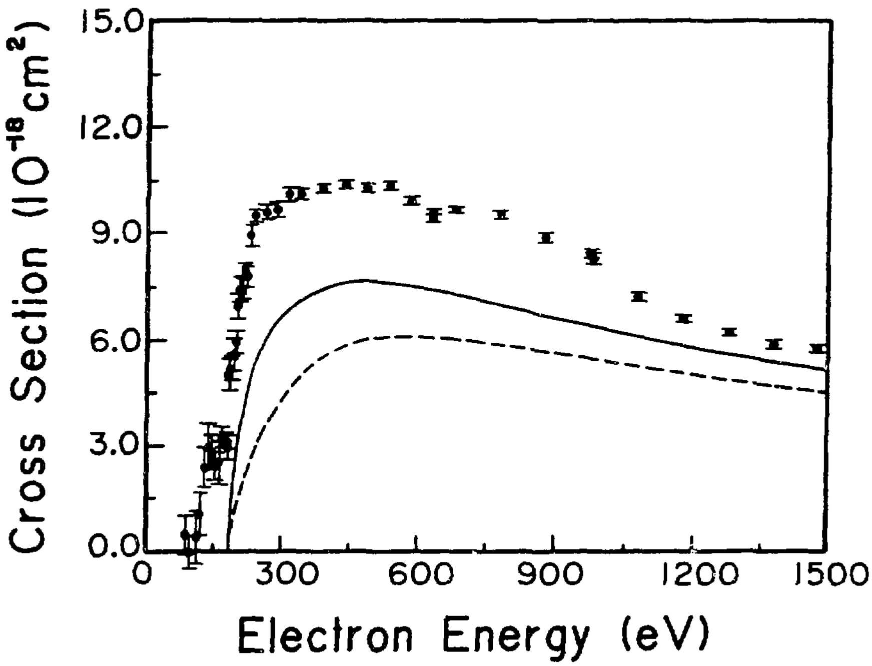

Figure 1
Electron-impact single ionization of Xe^{8+}. Solid curve, total cross section from the $4d^{10}$ ground configuration in the configuration-average distorted-wave method, Ref. 10; dashed curve, direct cross section only; solid circles, experimental measurements, Ref. 10.

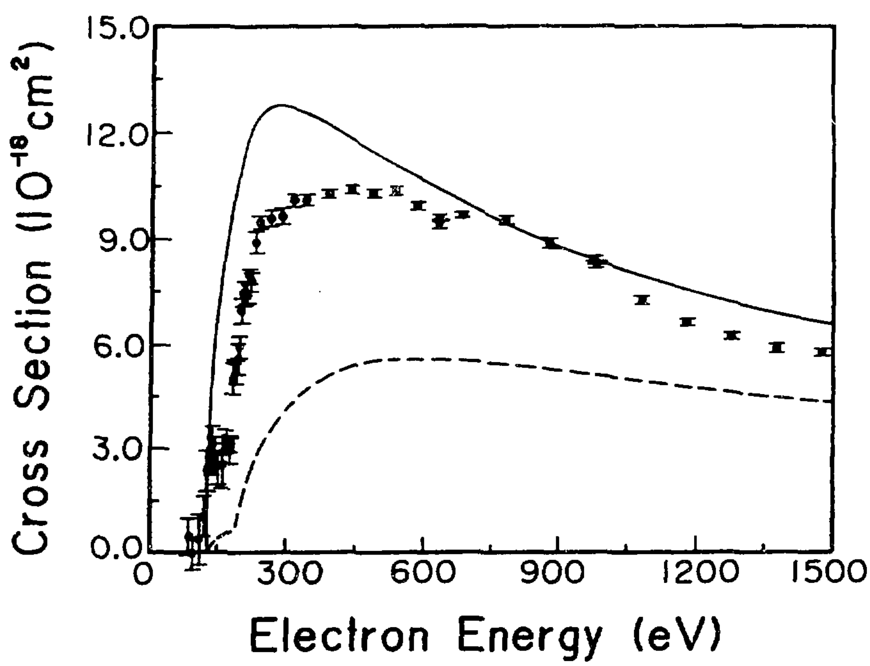

Figure 2.

Electron-impact single ionization of Xe^{8+}. Solid curve, total cross section from the $4d^95s$ excited configuration in the configuration-average distorted-wave method, Ref. 10; dashed curve, direct cross section only; solid circles, experimental measurements, Ref. 10.

In Fig. 2 the same experimental measurements are compared with configuration-average distorted-wave calculations for single ionization from the $4d^95s$ excited configuration of Xe^{8+}. The dashed curve is the sum of direct ionization cross sections for the 5s, 4d and 4p subshells. The largest excitation-autoionization contributions to the total ionization cross section come from the transitions 4d→5f, 4d→6d, 4d→6f, 4p→4f and 4p→5p. Although agreement between theory and experiment has improved in regard to the ionization threshold, the theoretical results are now substantially above the measurements at the cross section peak. We thus conclude that the ion beam has a substantial, but as yet unknown, metastable component. We note that a full level to level distorted-wave calculation for single ionization from an excited configuration of a heavy atomic ion may take a couple of orders of magnitude more CPU time than the corresponding configuration-average calculation. The increase in time scales roughly as the average number of levels per final configuration. For example the

4p→4f transition in Xe^{8+} results in a $4p^54d^94f5s$ final configuration which contains 226 levels.

In Fig. 3 experimental crossed-beams measurements[11] are compared with configuration-average distorted-wave calculations for double ionization from the $4d^95s$ excited configuration of Xe^{8+}. The ionization-autoionization contributions to the cross section come from direct ionization of the 4s, 3d, and 3p subshells. The direct double ionization contribution for Xe^{8+} is negligible. For double ionization from the $4d^{10}$ ground configuration, 4s subshell ionization-autoionization contributions are not energetically possible. Thus the reasonable agreement found between theory and experiment in the threshold region of Fig. 3 leads us to again conclude that the ion beam has a substantial metastable component. We note that for Xe^{8+} the peak double ionization cross section is about 6% of the peak single ionization cross section.

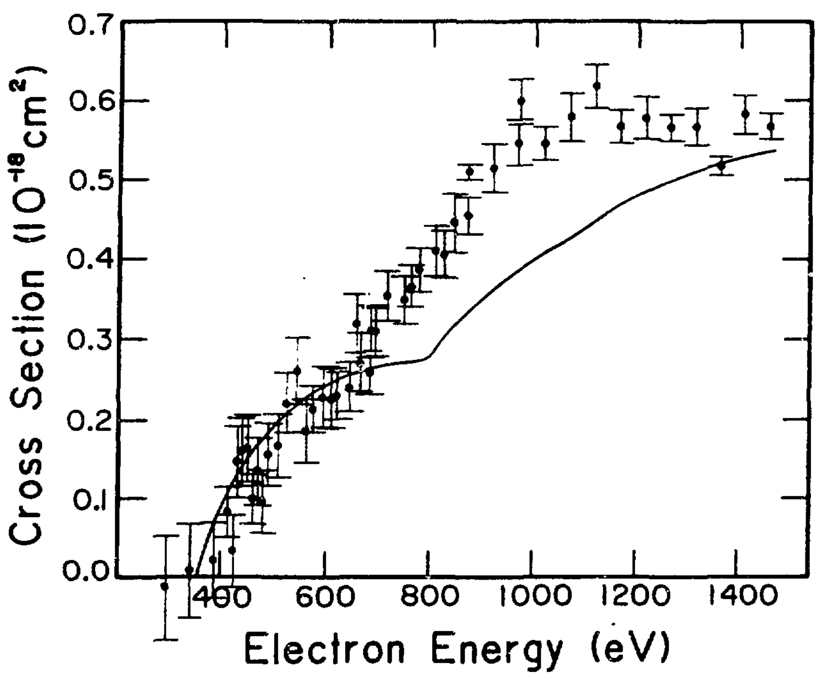

Figure 3.
Electron-impact double ionization of Xe^{8+}. Solid curve, total cross section from the $4d^95s$ excited configuration in the configuration-average distorted-wave method; solid circles, experimental measurements, Ref. 11

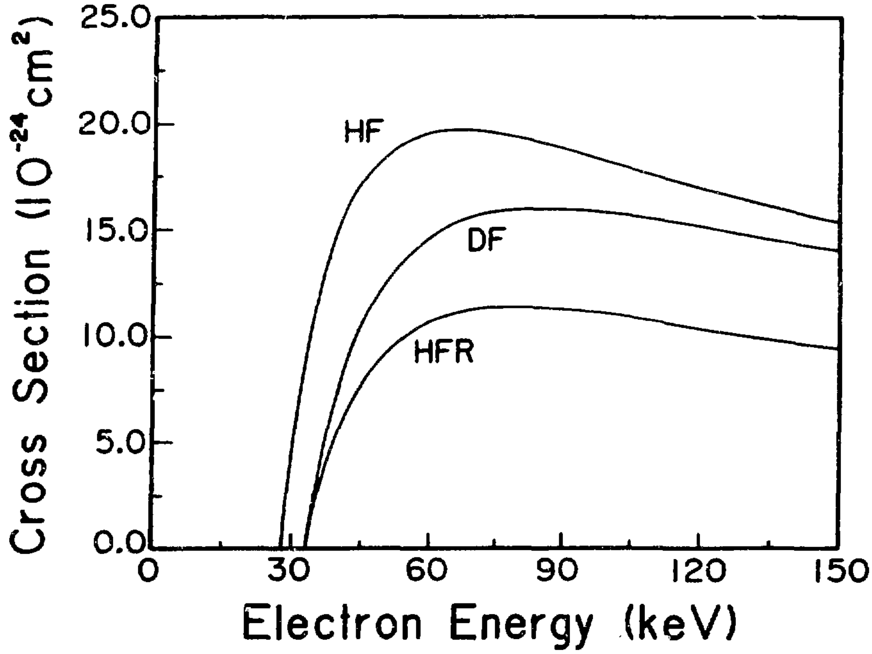

Figure 4.
Electron-impact ionization cross section for U^{89+}. The three solid curves are different approximations: Hartree-Fock (HF), Hartree-Fock with Relativistic-modifications (HFR) and Dirac-Fock (DF), Ref. 7.

For electron-impact ionization of heavy atomic ions, relativistic effects should play an important role. To explore the validity of semi-relativistic theories of ionization and to support LBL/ORNL channeling experiments using the Bevalac accelerator[12], we used the CAION and SCAION codes described in the third paragraph to calculate the 2s subshell ionization cross section for U^{89+}. In Fig. 4 electron ionization cross sections for U^{89+} are presented.[7] The HF and HFR results, which differ by almost a factor of 2 at the peak of the cross section, are both calculated using the CAION code. The semi-relativistic theory prediction of a decrease in the cross section is based, in part, on the relativistic contraction of the 2s target orbital. Based on the DF results calculated using the SCAION code, however, the semi-relativistic HFR theory has substantially overestimated the cross section reduction. The source of the major difference between the DF and HFR results can be traced to the neglect of the small component Dirac wavefunction inherent in the HFR method. We note that since the probability for radiative stabilization of the strongest inner shell excitations is high, that excitation-autoionization contributions to the total ionization cross section for U^{89+} are quite small.

We hope that this report on electron-impact ionization of heavy ions has given the reader a quick summary of this important subfield of electron scattering physics. In the future we look to improvements in crossed-beams experiments through both a better determination of the metastable content of the ion beam and an increase in the energy resolution of the electron beam. Experimental measurements on more highly charged systems should become available with the technological addition of both more powerful ion sources and heavy-ion storage rings. Exciting theoretical problems remain in trying to obtain a better understanding of (1) the three-body problem in direct ionization, (2) continuum-coupling effects in excitation-autoionization, (3) interference effects among various indirect ionization processes, and (4) plasma density effects on electron ionization.

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