Electron-impact double-ionization cross sections for Xe^{8+}

D. W. Mueller
Department of Physics, University of North Texas, Denton, Texas 76203

L. J. Wang* and D. C. Gregory
Physics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6372

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Absolute cross-section measurements are presented for the double ionization of Xe^{8+} by electron impact from below threshold to 1500 eV. A search for direct double ionization indicates that this process is small or negligible compared to the single-electron processes which contribute to double ionization. The presence of a high percentage of metastable target ions in the interaction region of this experiment significantly affects the interpretation of the measured cross sections and indicates the potential importance of selected metastable ions in plasmas.

One of the more intriguing aspects of electron-impact ionization is the inherent difficulty of theory to handle few-body (three- or more-body) problems. For multiple ionization this difficulty becomes a virtual impossibility unless some simplifying assumptions can be made. The most commonly applied model for direct double ionization is the semiclassical binary-encounter approximation (BEA).[1] Predictions based on this model have been compared to measurements for direct multiple ionization of argon ions[2,3] and of xenon ions.[4-6] These comparisons indicate that when significant excitation or ionization from the inner shells of the target ion occurs, direct double ionization, which is a second-order process, generally contributes less to the cross section than indirect first-order processes such as excitation–double-autoionization or ionization-autoionization. Our intent here was to provide some additional insight into the relative probabilities of direct and indirect double-ionization processes.

We have measured the cross section for electron-impact double ionization of Xe^{8+}. Xenon is one of the most comprehensively studied isonuclear series in the field of electron-impact ionization,[4-8] and data are available for single ionization of xenon ions in initial charge states 1+ through 8+. Measured and calculated cross-section curves have revealed rich and varied structures and strong term dependence in excitation of the $4d$ subshell.[5,9-11] Previous measurements indicate that an important mechanism for double ionization in the lower charge states of the xenon isonuclear series is the direct ionization of a single inner-shell $4d$ electron followed by autoionization of the resulting excited ion.[4-6] The relative contribution of direct double ionization to the total double-ionization cross section is expected to decrease in comparison with $4d$ ionization-autoionization with increasing target-ion charge as more of the $n=5$ shell electrons are removed (leaving fewer outer-shell electrons) and as the binding energy of the outer electrons increases (decreasing the overall probability of ionization). Since the $4d$ electrons form the outer shell of ground state $Xe^{8+}(4s^2 4p^6 4d^{10})$, $4d$ ionization-autoionization is no longer possible and, because of the large number of outer-shell electrons (ten) present, we may expect to detect direct double ionization.

Figure 1 is an energy-level diagram showing the average energies [calculated using Cowan's relativistic Hartree-Fock (RHF) code[12]] of selected configurations for Xe^{8+} through Xe^{11+} with the ground state of Xe^{8+} taken as the reference energy. Energetically, the threshold for direct double ionization from the ground state of Xe^{8+} is 385 eV (transition $1D$ in Fig. 1). As can be seen in the figure, the lowest-energy one-electron process which is expected to contribute to double ionization of ground-configuration Xe^{8+} is excitation of an inner-shell $3d$ electron to the $n=5$ shell (transition $1B$), which has a threshold energy of 675 eV. This excitation is followed by subsequent double-autoionization (transitions $3A$ and $4A$) or auto-double-ionization (transition $3B$).[13] Thus we

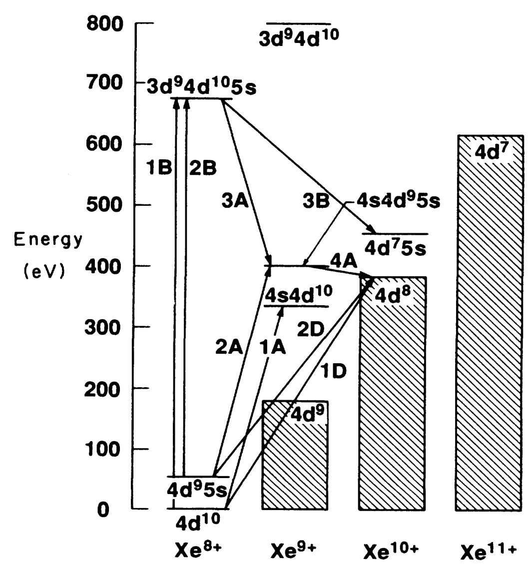

FIG. 1. Selected configuration-average energies of Xe^{8+} through Xe^{11+}, calculated with the relativistic Hartree-Fock code by Cowan (Ref. 12).

might expect the cross section in the energy range between 385 and 675 eV to be due only to direct double ionization. With these concepts in mind we proceeded with measurements of the cross section for the double ionization of Xe^{8+}.

The experimental arrangement has been previously described in the literature,[14] so only a brief presentation will be given here. The measurements utilized beams of ions extracted from the Oak Ridge National Laboratory Electron Cyclotron Resonance ion source[15] and electrons from a gun described by Taylor *et al.*[16] intersecting at right angles. The beam overlaps are measured along with the primary-beam currents and the efficiency of detection of the signal ions. The ionized ions are separated from the primary beam by a magnetic analyzer and the ions with a higher charge are counted for a given time interval. From this information the absolute electron-impact ionization cross section may be determined at each interaction energy. The absolute uncertainty for a typical measurement near the peak cross section (including statistics) is approximately 8% at a 90% confidence level, equivalent to two standard deviations for statistics.

The measured cross section versus incident electron energy for double ionization of Xe^{8+} is shown in Fig. 2 with the associated numerical values presented in Table I. Uncertainties in the table and figure reflect relative uncertainties only (dominated by the counting statistics) at a level equivalent to one standard deviation on statistics only. Two features are immediately apparent in the graph. First, the threshold for double ionization lies at or below 400 eV. Second, the cross-section curve follows an apparent straight line on this linear plot from the observed threshold to 1000 eV. A threshold energy less than 385 eV would indicate a metastable content in the

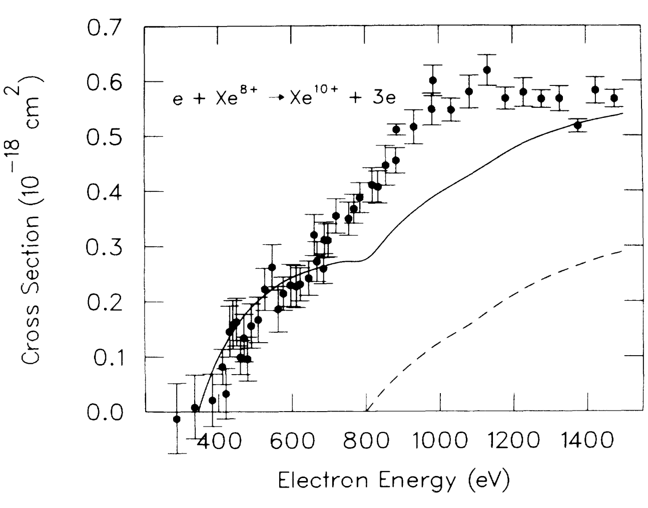

FIG. 2. Cross sections for double ionization of Xe^{8+}. The circles are the present data, with one-standard-deviation relative uncertainties. The absolute uncertainty for a typical point near the peak of the cross section is ±8%. The solid line is the Lotz prediction for ionization autoionization of 4*s*, 3*d*, and 3*p* electrons from metastable Xe^{8+} ($4d^95s$). The dashed curve is the Lotz prediction for ionization of 3*d* and 3*p* electrons from the ground state of Xe^{8+}.

beam (a linear extrapolation indicates a threshold near 340 eV). The double-ionization threshold from the lowest metastable configuration, $4d^95s$, is 327 eV (transition 2*D* in Fig. 1). The lowest-energy one-electron process which will lead to double ionization (ionization of a 4*s* electron followed by autoionization—transitions 2*A* and 4*A*) lies only 344 eV above the $4d^95s$ metastable state. The mea-

TABLE I. Cross-section measurements for double ionization of Xe^{8+} by electron impact. Uncertainties are relative only, at the one-standard-deviation confidence level.

Energy (eV)	Cross section (10^{-18} cm^2)
286	−0.013±0.065
335	0.008±0.059
383	0.021±0.048
411	0.082±0.032
420	0.033±0.046
431	0.146±0.046
440	0.158±0.044
450	0.163±0.043
460	0.099±0.031
470	0.134±0.043
479	0.096±0.040
490	0.156±0.040
509	0.167±0.041
527	0.222±0.038
547	0.262±0.041
563	0.186±0.041
577	0.214±0.030
597	0.229±0.038
612	0.227±0.038
623	0.231±0.030
646	0.242±0.031
661	0.320±0.037
668	0.272±0.036
686	0.259±0.027
688	0.311±0.032
698	0.310±0.030
720	0.354±0.031
754	0.349±0.030
768	0.367±0.026
784	0.387±0.027
817	0.410±0.031
833	0.406±0.029
854	0.445±0.036
882	0.454±0.023
884	0.510±0.010
931	0.515±0.031
980	0.547±0.029
984	0.599±0.028
1032	0.546±0.021
1082	0.579±0.030
1131	0.618±0.028
1180	0.567±0.020
1229	0.578±0.026
1278	0.566±0.016
1327	0.567±0.023
1376	0.517±0.012
1425	0.582±0.024
1476	0.567±0.016

sured threshold, then, is consistent with either direct or indirect double ionization from the metastable level as well as direct double ionization from the ground state. It should be noted that direct single ionization from the $4s$ subshell of the ground state (transition $1A$, leading to Xe^{9+} $4s4d^{10}$) lies below the autoionization threshold and will not lead to a double-ionization event, while the corresponding transition in the metastable ion (transition $2A$) does lead to a state which can autoionize.

The solid line in Fig. 2 is the cross section calculated for the ionization-autoionization process from the $4d^95s$ metastable configuration of Xe^{8+} using the semiempirical Lotz formula[17]

$$\sigma=\sum_j \frac{(4.5\times10^{-14})r_j\ln(E/I_j)}{EI_j}H(E-I_j)\ , \qquad (1)$$

$$H(X)=\begin{cases}0 & \text{if } X<0\\ 1 & \text{if } X>0\ .\end{cases}$$

The cross section σ (in cm^2) at an energy E (in eV) for a set of subshells j depends only on the subshell ionization potentials I_j and the number of electrons r_j in each subshell. Ionization from the $4s$, $3d$, and $3p$ subshells have been included. Although Xe^{9+} ions with vacancies in the $3d$ or $3p$ subshells have sufficient energy to double autoionize and could result in a net triple-ionization event, the dominant branching paths from these excited states are expected to result in a net double-ionization event. The dashed curve in Fig. 2 is the Lotz prediction for ionization-autoionization from the $3d$ and $3p$ subshells of the ground configuration of Xe^{8+}. The presence in the ion beam of any metastable component obviously will greatly affect the measured cross section. A similar dramatic dependence on the metastable fraction was observed[8] in single ionization of Xe^{8+}.

The other significant indirect process which could contribute to this cross section is the excitation of an inner electron followed by double autoionization. The first excitation transition which could contribute to double ionization from a metastable ion is $3d$-$4d$ excitation (transition $2B$), which has a threshold at about 618 eV. The $3d$-$5p$ transition onsets less than 25 eV higher, and a whole series of transitions involving the $3d$ or $3p$ electrons extends to higher energies. The contributions of these processes to the measured total cross section depends on the excitation cross sections and the branching probabilities of the resulting excited states for each individual transition. Although we cannot accurately assess their importance in this case, contributions from excitation-autoionization are often important or even dominant in ionization measurements. The shape of the curve below 1000 eV implies that numerous transitions with thresholds between 618 and 1000 eV may each contribute a small amount to the measured cross section. This is consistent with the fact that each of the configurations shown in Fig. 1 is an average of a large manifold of states.

The reasonable agreement between the experimental data and the Lotz prediction for metastable ions below 700 eV suggests that the single-electron indirect process of ionization-autoionization dominates double ionization of metastable Xe^{8+}. Excitation–double-autoionization may account for some of the additional observed cross section. We are unable to determine the importance of direct double ionization in this measurement due to uncertainties in the metastable fraction of the incident ion beam and in the contribution of excitation–double-autoionization to the total cross section. The observation of a large metastable component in the ion beam (despite the estimated 10-ms time of flight from the ion source to the collision region) underscores the possible presence of excited ions in ion sources and plasmas. The dramatic effect of the metastable ions on the measured cross sections in this experiment suggests that, although plasma conditions vary, some excited states of ions are long lived and it may be necessary to include this possibility in plasma modeling.

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*Present address: Department of Physics and Astronomy, Vanderbilt University, Nashville, TN 37235.

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