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FORMATION OF IONIZED EXCITED STATES FROM THE LOSS OF THE METASTABLE ELECTRON IN THE NOBLE GAS ATOMS

DRF-4871

S.H. Koozekanani

The Ohio State University

ElectroScience Laboratory

(formerly Antenna Laboratory)
Department of Electrical Engineering
Columbus, Ohio 43212

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ABSTRACT

It is shown that when the metastable electron of a noble gas atom is removed by a fast collision it is quite possible for the atom to be ionized and excited at the same time. Excitation cross sections for the processes $np^5 - (n+1)s \xrightarrow{-s} np^4 - m\ell''$ or $np^5 - (n+1)s \xrightarrow{-p} np^4 - m\ell''$ have been calculated in terms of the cross sections for removing the electrons.

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I. INTRODUCTION

In some discharge situations, we can think that the atom is first excited to a metastable state and then, through collision with another electron, the atom loses its metastable electron and becomes ionized. This situation is to some extent favored over the direct one step ionization. For example, for neon the ionization cross section threshold from the ground state is 21.5 eV. whereas from the metastable $2p^5 - 3s$ state it is just about 5 eV. Since there are more electrons available at the lower energies than at the higher 21.5 eV. range, it is more probable to ionize the atom from its long lived metastabel state than from the ground state; however, this depends upon the population of the metastable states in the particular discharge.

The atom in its metastable state has quite a large cross sectional area since the excited electron has a classical orbit which is extended away from the center of the atom. For example $\langle r_{4s} \rangle_{av.}$ for the 4s electron of ArI $3p^5$-4s is 14.67 A.U., whereas the corresponding 3p electron has an $\langle r_{3p} \rangle_{av.} = 4.2$ A.U. It can be assumed that it is much easier to remove the 4s metastable electron than one of the $3p^6$ electrons of AI, since it offers a bigger cross section and is more loosely bound.

The question which one can now ask is what happens when the metastable electron of a noble gas atom is removed in a very short time compared to the relaxation time of the ion. Is it possible for the atom to go to an ionized excited state by just losing its metastable electron, or in equation form, is it possible to have, Fig. 1

(1) $$np^5 - (n+1)\,s \xrightarrow{-(n+1)\,s} np^4 - m\ell'$$

where ℓ' is the angular quantum number of the excited electron and m is its principle quantum number? Moreover, for the sake of the argument, what happens if an np electron is lost in a very short time, i.e., Fig. 2

(2) $$np^5 - (n+1)\,s \xrightarrow{-np} np^4 - m\ell$$

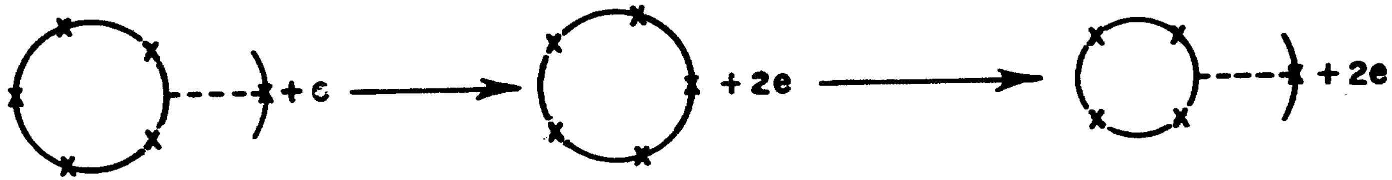

FIGURE 1

Here the metastable electron of a noble gas atom is lost through collision and the atom becomes simultaneously ionized and excited, i.e., $p^5 - ns \xrightarrow{-ns} p^4 - mp$.

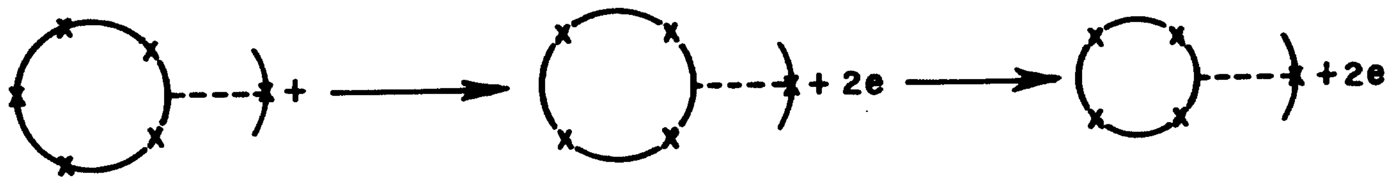

FIGURE 2

Here one of the ground state valence electrons is lost through collision and the atom becomes ionized and excited, i.e., $p^5 - ns \xrightarrow{-e} p^4 - ms$.

In Sections II and III of this work, we shall calculate probabilities for these processes in terms of the cross sections for removing these electrons.

II. THE METASTABLE ATOM MINUS s-ELECTRON

When the metastable noble gas atom with configuration np^5 - $(n+1)s$ loses its s-electrons, it is left in a np^5 state. To write this in a more formal way, we have,

$$(3) \qquad \left| \ell_0^5\, L'S'J', n\ell', K, s, JM \right> \xrightarrow{-s} \left| \ell^5\, L'S'J'M' \right>$$

For the two metastable states of noble gas atoms we have $J = 2$, $K = 3/2$, $J' = 3/2$ and $J = 0$, $K = 1/2$, $J = 1/2$ with ℓ 0 and $\ell = \ell_0 = 1$.

To calculate the cross section for the process of Eq. (3) when the s-electron is stripped away in a very short time, we expand the initial state[1] which is the product of a metastable atom and a free electron in terms of the final states which are the products of an ejected electron, a free electron, and an ionized atomic state of the form $np^4 - n\ell'$. In other words,

$$(4) \qquad \left| \ell^5\, L'S'J', n\ell', K, s\, J_0 M_0 ; k_i \right> = \sum_{n,f} a_n \left| \ell^4\, \overline{L}\,\overline{S}, n\ell'' s,\ LSJM; \; k_{1f}\, ; E\ell_f \right>$$

where, $|k_i>$, $|k_{1f}>$ and $|E_2 \ell_f>$ are the wavefunctions of the initially free and the ejected electrons. From Eq. (2) we have,

$$(5) \qquad a_{mf} = \left< \ell^4 \overline{L}\,\overline{S}, m\ell'' s,\ L\,S\,J\,M{:}k_{1f};\ E\ell_f \right| \left. \ell_0^5\ \ L'S'J', \ell', K, s\,J\,M \right>$$

$$= \sum_{M_k, m_s, m_{\ell'}, M'} \left< \ell^4 \overline{L}\,\overline{S},\ m\,\ell'' s,\ L\,S\,J\,M \right| \left. \ell_0^5\, L'S'J'M' \right>$$

$$\begin{pmatrix} K & s & J_0 \\ M_K & m_s & -M_O \end{pmatrix} \begin{pmatrix} J' & \ell' & K \\ M' & m_{\ell'} & -M_k \end{pmatrix} \left< k_{if} | k_i \right> \left< E\ell_f | \ell' m_\ell' \right>$$

$$(2J_0+1)^{\frac{1}{2}}\, (2K+1)^{\frac{1}{2}}\, (-1)^{K - s + M + J' - \ell' + M_k}$$

or

(6) $$a_{mf} = (\ell^4 \bar{L}\bar{S}\ \{| \ell_0^5\ \acute{L}\acute{S})\ F_4(\ell_0, \ell)\ F_1(\ell_0, m\ell'')\ \delta(J, \acute{J})\ \delta(\ell_0, m\ell')$$

$$\sum_{M_k m_s m'} \begin{pmatrix} K & S & J \\ M_k & m_s & -M \end{pmatrix} \begin{pmatrix} J & \ell' & K \\ \acute{M} & m & -M_k \end{pmatrix} \langle k_{if} | k_i \rangle \langle E\ell_f | n\ell m_\ell \rangle$$

$$(2J_0 + 1)^{\frac{1}{2}}\ (2K + 1)^{\frac{1}{2}}\ (-1)^{K - s + M + \acute{J} - \ell' + M_k}$$

where

(7) $$F_4(\ell_0, \ell) = \left[\int_0^\infty R_{\ell_0}(r)\ R_\ell(r)\ r^2\ dr\right]^4$$

(8) $$F(\ell_0, m\ell'') = \int_0^\infty R_{\ell_0}(r)\ R_{\ell''}(r)\ r^2\ dr$$

and we have assumed that the inner orbitals remain unchanged after ionization. $R_\ell(r)$ is the radial portion of the single electron wave-function with $(\ell^4\ \bar{L}\bar{S}\ \{| \ell^5\ \acute{L}\ S)$ being the usual coefficient of fractional parentage.[2]

The probability that the atom after losing its metastable electron is in an excited ionized state of the form $|\ell^4\ \bar{L}\bar{S}, m\ell''s, L\ S\ J\ M\rangle$ is proportional to

$$\left| \sum_f a_{nf} \right|^2$$

and the cross section for such a process would be

(9) $$Q_{m\ell''}(E) = (\ell^4\ \bar{L}\bar{S}\ \{| \ell^5\ \acute{L}\ \acute{S})^2\ F_4^2(\ell_0, \ell)\ F_1^2(\ell_0, m\ell'')\ Q_s(E)\ \delta(\ell_0, m\ell'')$$

$Q_s(E)$ is the cross section for removing the s electron from the $np^5 - (n+1)s$ atomic configuration. This cross section has a threshold of about 4 eV for argon and should be about an order of magnitude larger than the simple ionization cross section, since the metastable electron is farther removed from the center of the atom. Table I gives the product of $F_4(\ell, \ell_0)\ F_1(\ell_0, m\ell'')$ for neon, argon and krypton and Table II gives the cross sections for some of the $3p^4$-$4p$ states of argon II in terms of $Q_{4s}(E)$.

III. THE METASTABLE ATOM MINUS p-ELECTRON

We assume the atomic configuration $np^5 - (n+1)\,s$ loses one of its np electrons in a fast collision. The cross section for the process should be of the same order of magnitude as the ionization cross section from the np^6 state under the same conditions. Before removing the np electron we have to make a change of coupling from $np^5 - (n+1)\,s$ to $|[np^4, (n+1)\,s] - np>$. This will enable us to know what states will be allowed to exist. The neutral noble gas atoms are given in the pair coupling scheme. We first write these states in terms of LS coupled states; here for the metastable states we notice that we have

$$(10)\qquad |\ell_0^5\, L'S'J'; \ell', K.\, S\, J = {}^{2}_{0},\, M> \;=\; |\ell_0^5\, L'S', \ell s,\, L = 1\ \ S=1,\ J = {}^{2}_{0}, M>$$

$$= \sum_{\psi_2} \sum_{L_1 S_1} \sum_{j\, J''} (-1)^{L'+L_1+\ell_0+\ell'+S'+S_1+2s_1} (\ell^5\, L'S'\{|\ell^4\, \overline{L}\, \overline{S})$$

$$\{[L']\,[S']\,[L]^2\,[S]^2\,[J]\,[j]\}^{\frac{1}{2}} \begin{Bmatrix} L & \ell_0 & L' \\ L & \ell' & L_1 \end{Bmatrix} \begin{Bmatrix} S & s & S' \\ S & s & S_1 \end{Bmatrix} \times$$

$$\begin{Bmatrix} L_1 & \ell_0 & L \\ S_1 & s & S \\ J_1 & j_0 & J \end{Bmatrix} |(\ell_0^4\ \overline{L}\,\overline{S}\ n\ell' s)\ L_1 S_1 J_1,\ (\ell_0 s)\ j_0, J\, M>$$

where the symbol $[x] = 2x + 1$.

To find the cross section we expand the state $|\ell_0^4 \overline{L}\,\overline{S}, n\ell' s)\, L_1 S_1 J_1,$ $(\ell_0 s)\ j_0, J\ M; k_i>$ which is the product of an atomic state and a free electron k_i in terms of the final state which are a product of the excited ionic states

$|\ell^4 \bar{L}\,\bar{S}, m\ell''s,\ L_k\, S_k\, J_k\, M_k\rangle$ and a free and an ejected electronic state. The new atomic states are exactly the states in the right-hand side of Eq. (10) minus the ℓ, s electron. After some algebra similar to that of Section I we obtain for the cross section,

$$(11)\qquad Q(|\ell^4 \bar{L}\,\bar{S}, m\ell''s,\ L_k\, S_k\, J_n\, M_k\rangle = Q_{\ell_0}(E)\,(\ell^5,\, L'\, S'\{|\ell^4 \bar{L}\,\bar{S})^2$$

$$[L'][S'][L]^2[S]^2 \begin{Bmatrix} L & \ell_0 & L' \\ L & \ell' & L_1 \end{Bmatrix}^2 \begin{Bmatrix} S & s & S' \\ S & s & S_1 \end{Bmatrix}^2 F_4^2(\ell_0, \ell)\, F_\ell^2(n\ell', m\ell'')$$

$$\sum_{j_0} [J_1][j_0] \begin{Bmatrix} L_1 & \ell_0 & L \\ S_1 & s & S \\ J_1 & j & J \end{Bmatrix}^2 \delta(n\ell', m\ell'')$$

We notice here that the possible excited states are of the form p^4-ms, i.e., the excited electron should be an s-electron.

Table III gives the product of $F_4(\ell_0, \ell)\, F_1(n\ell', m\ell'')$ for argon, neon and krypton and Table IV gives the cross section for some of the states of $3p^4$-ms of argon II the metastable states J = 0 and J = 2.

To obtain the radial wavefunctions, a Hartree Fock self-consistent computer program in the Slater approximation given by Herman and Skilman[2] was used and a computer was used to obtain the radial integrals.

IV. CONCLUSIONS

One sees in these calculations that if the loosely bound metastable s-electron of NeI, ArI or KrI is suddenly removed, the remaining atom is perturbed enough to repel one of its np electrons to an excited shell with fairly good probability.

TABLE I
PRODUCT OF $F_4(\ell_0, \ell)\ F_1(\ell_0, n\ell'')$
FOR NEON, ARGON AND KRYPTON

$n\ell''$	2p	3p	4p	5p	6p	7p	8p
Neon	0.995	-0.049	-0.0246	-0.0138	-0.009	---	---
Argon	---	0.995	-0.047	-0.0233	-0.0134	-0.0087	---
Krypton	---	---	0.995	-0.048	-0.0232	-0.0132	-0.0085

TABLE II
EXCITATION CROSS SECTION FOR SOME OF THE ArII STATES WHEN $3p^5$-4s METASTABLE STATE LOSES ITS s-ELECTRON IN A FAST COLLISION. ALL ArII p^4-4p STATES WITH $\bar{J}=3/2$ AND $\bar{J}=1/2$ ARE MIXED.[4] EQUATION (13) IN REFERENCE 5 WAS USED TO CALCULATE THE ABOVE RESULTS

Possible $3p^4$-4p states	$\frac{Q(E)}{Q_{4s}(E)}$ for both the $3p^5$-4s metastables with J=2 and J=0
$p^4[3p]$ - 4p $^2S_{1/2}$	0.109×10^{-3}
$p^4[3p]$ - 4p $^2P_{1/2}$	0.351×10^{-3}
$p^4[3p]$ - 4p $^2P_{3/2}$	0.406×10^{-3}
$p^4[3p]$ - 4p $^2D_{3/2}$	0.198×10^{-3}
$p^4[3p]$ - 4p $^4P_{3/2}$	0.002×10^{-3}
$p^4[3p]$ - 4p $^4D_{3/2}$	0.002×10^{-3}
$p^4[3p]$ - 4p $^4S_{3/4}$	0.006×10^{-3}
$p^4[3p]$ - 4p $^4P_{1/2}$	0.001×10^{-3}
$p^4[^1D]$ - 4p $^2P_{3/2}$	1.444×10^{-3}
$p^4[^1D]$ - 4p $^2P_{1/2}$	1.529×10^{-3}
$p^4[^1D]$ - 4p $^2D_{3/2}$	0.002×10^{-3}

TABLE III

THE PRODUCT OF $F_4(\ell_0, \ell)\,F(n\ell', m\ell'')$ FOR NEON n=3, FOR ARGON n=4 AND FOR KRYPTON n=5

$m\ell''$	3s	4s	5s	6s	7s	8s
Neon	0.904	-0.439	-0.075	-0.044		
Argon	---	0.920	-0.425	-0.068	-0.041	
Krypton	---	---	-.926	-0.416	-0.067	-0.040

TABLE IV

EXCITATION CROSS SECTION FOR THE $3p^4$-4s STATES OF ARGON II

$3p^4$-4s possible states	$\frac{Q(E)}{Q_{3p}(E)}$ from $4s'\left[\frac{1}{2}\right]_0$	$\frac{Q(E)}{Q_{3p}(E)}$ from $4s\left[\frac{3}{2}\right]_2$
$3p^4\,[^1S]\ 4s\ ^2S_{1/2}$	0.012	0.012
$3p^4\,[^3P]\ 4s\ ^2P_{1/2}$	0.024	0.002
$3p^4\,[^3P]\ 4s\ ^2P_{3/2}$	0.040	0.010
$3p^4\,[^3P]\ 4s\ ^4P_{1/2}$	0.016	0.005
$3p^4\,[^3P]\ 4s\ ^4P_{3/2}$	0.080	0.027
$3p^4\,[^3P]\ 4s\ ^4P_{5/2}$	0.0	0.064
$3p^4\,[^1D]\ 4s\ ^2D_{1/2}$	0.060	0.006
$3p^4\,[^1D]\ 4s\ ^2D_{1/2}$	0.0	0.054

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