Electron impact excitation of the \(5p^77p\) levels of xenon from \(5p^56s\) metastable states

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Abstract

Relativistic distorted-wave (RDW) calculations have been carried out for the electron impact excitation from the lowest metastable states of xenon (the \(J = 0, 2\) levels of the \(5p^56s\) configuration) to the ten higher-lying fine-structure levels of the \(5p^77p\) configuration. Integrated cross section results are reported for incident electron energies up to 300 eV and their analytic fits are also provided for obtaining results at higher energies.

1. Introduction

The importance of electron impact excitation cross sections from the lowest metastable levels of the inert gases, i.e. the \(J = 0, 2\) levels of the \(np^5(n+1)s\) configuration to all ten fine-structure levels of the \(np^5(n+2)p\) configurations (with \(J = 0, 1, 2\) and 3) has been repeatedly emphasized [1-4]. Experimental work to study excitations of the \(np^5(n+2)p\) configurations is in progress by the Wisconsin Group. They recently reported experimental results for argon [2] and we have carried out relativistic distorted-wave (RDW) calculations for these excitations [3]. In the present brief report we consider similar excitations in xenon in the light of further ongoing measurements. Results for such excitations in xenon have also been in demand as these contribute significantly to plasma modeling, in particular for plasma diagnostic of xenon-fed thrusters [4,5]. The role and effect of our calculated cross section in the plasma diagnostic of these thrusters is currently under way using a collisional radiative model (CRM).

We report here detailed results from our RDW calculations to obtain the integral cross sections (ICS) for the fine-structure transitions in xenon from the \(5p^56s\) metastable levels to the higher lying fine structure levels of \(5p^77p\) configurations. The details of the theoretical calculations of the cross sections have been given in our earlier publications [1,3]. In the next section we describe the results for the atomic target wave functions of xenon. Section 3 presents our ICS results and their analytic fits.

2. Wave Functions

The ground state of xenon has a \(5p^6\) outer shell in the nonrelativistic representation. Since we are using the relativistic \(j-j\) coupling scheme, the \(5p^5\) core of the excited states is split into two separate configurations, \(5\overline{p}5p^7\) and \(5\overline{p}5p^7p^3\), with total angular momenta \(j\), of 1/2 and 3/2, respectively. The lowest lying metastable states of xenon with total angular momentum \(J = 2\) and \(J = 0\) (designated as \(1s_{5}\) and \(1s_{3}\), respectively, in the Paschen notation) have the configurations \(5\overline{p}^25p^36s\) and \(5\overline{p}5p^66s\) in the \(j-j\) coupling scheme. Thus the hole in the valence shell is different for these two metastable states.

We are considering the electron impact excitation to the ten individual fine-structure levels of the \(5p^77p\) manifold. In the \(j-j\) coupling scheme, these states are linear combinations of the configurations \(5\overline{p}25p^37\overline{p}\) with \(J = 1, 2\); \(5\overline{p}5p^7p\) with \(J = 0, 1, 2, 3\); \(5\overline{p}5p^77\overline{p}\) with \(J = 0, 1\) and 5 \(\overline{p}5p^77p\) with \(J = 1, 2\). In the Paschen notation, the fine-structure levels are denoted as \(3p_{i}\) where \(i\) varies from 1 to 10.

We have used the GRASP92 program [6] to obtain Dirac-Fock target-state wave functions for Xe which produced good agreement with the measured values of the oscillator strengths for these transitions.
where available. Our calculated dipole oscillator strengths for 1s\textsubscript{5}-3p\textsubscript{i} and 1s\textsubscript{5}-3p\textsubscript{k} transitions are 2.30\times10\textsuperscript{-3} and 4.60\times10\textsuperscript{-3} compared with the values available from NIST database (http://physics.nist.gov/PhysRefData/ASD/index.html) of 2.67\times10\textsuperscript{-3} and 5.86\times10\textsuperscript{-3} respectively. The estimated error in NIST values is 50% and oscillator strengths are available only for these two transitions. Table 2 shows our calculated excitation energies for different transitions as compared to the NIST values and can be said to be in reasonable agreement.

The contributions from the various configurations to the fine-structure levels of the final states are given in table 2. The 3p\textsubscript{k} level with J = 3 has the single configuration 5\( \overline{p} \)^25p\textsuperscript{3}7p. Note that we have not calculated wave functions for the 3p\textsubscript{i} level with J = 0 in Xe. This level with an excitation energy of 22.23 eV lies much above the first ionization potential of 12.13 eV for Xe and therefore accurate representation of this level cannot be achieved within a Dirac-Fock approximation without including mixing with the continuum. We observe that with the exception of the 3p\textsubscript{i} and 3p\textsubscript{10} levels these states are overwhelmingly dominated by a single configuration and that these two exceptions come from a single core with a \( \overline{p} \) hole.

Table 1: Excitation energies of various transitions in Xe

| Transition   | GRASP | NIST       |
|--------------|-------|------------|
| 1s\textsubscript{5}-1s\textsubscript{3} | 1.30104 | 1.13188   |
| 1s\textsubscript{5}-2p\textsubscript{10} | 1.85745 | 2.58626   |
| 1s\textsubscript{5}-2p\textsubscript{9} | 1.90877 | 2.63890   |
| 1s\textsubscript{5}-2p\textsubscript{8} | 1.90529 | 2.65347   |
| 1s\textsubscript{5}-2p\textsubscript{7} | 1.95456 | 2.68041   |
| 1s\textsubscript{5}-2p\textsubscript{6} | 1.94552 | 2.68761   |
| 1s\textsubscript{5}-2p\textsubscript{5} | 2.04625 | 2.69972   |
| 1s\textsubscript{5}-2p\textsubscript{4} | 3.22909 | 3.94118   |
| 1s\textsubscript{5}-2p\textsubscript{3} | 3.25242 | 3.96758   |
| 1s\textsubscript{5}-2p\textsubscript{2} | 3.24499 | 3.96568   |

Table 2: Contributions of the various configurations to the 5p\textsuperscript{3}7p states of Xe

| Configurations     | J = 0 levels | J = 1 levels | J = 2 levels |
|--------------------|--------------|--------------|--------------|
|                    | 5p\textsubscript{3} | 3p\textsubscript{2} | 3p\textsubscript{3} | 3p\textsubscript{6} | 3p\textsubscript{9} |
|                    | 0.9976       | 0.0011       | 0.017        | 0.0421        | 0.9577        |
|                    | 0.0024       | 9.37\times10\textsuperscript{-4} | 4.36\times10\textsuperscript{-5} | 0.9579        |
|                    | 9.37\times10\textsuperscript{-4} | 4.25\times10\textsuperscript{-4} | 2.76\times10\textsuperscript{-4} | 8.84\times10\textsuperscript{-5} |

3. Results and Discussions

We present cross sections for the electron impact excitation of xenon from the 1s\textsubscript{3} and 1s\textsubscript{5} metastable levels to the fine-structure levels of the 5p\textsuperscript{3}7p manifold (designated as 3p\textsubscript{i}, i = 2 - 10). Figure 1 displays the cross sections for these transitions in the energy range up to 300 eV. In figures 1(a) and 1(b) we show the results for the dipole allowed transitions where the final states have respectively a \( \overline{p} \) or \( p \) hole in the valence shell. A transition from the 1s\textsubscript{3} level with configuration 5\( \overline{p} \)^25p\textsuperscript{3}6s and \( j_c = 3/2 \) to a level whose wave functions are comprised almost entirely of configurations 5\( \overline{p} \)^25p\textsuperscript{3}7p with \( j_c = 1/2 \) represents a two-electron transition. For such transitions cross section would be expected to be smaller compared to those from the 1s\textsubscript{3} level with configuration 5\( \overline{p} \)5p\textsuperscript{4}6s. This can be clearly seen in figure 1(a). Likewise, excitations of levels with wave functions dominated by the 5\( \overline{p} \)^25p\textsuperscript{3}7p configuration with \( j_c = 3/2 \) from the 1s\textsubscript{3} level would be expected to have smaller cross sections than those for excitations from the 1s\textsubscript{5} state as shown in figure 1(b). Similar behaviour was shown to be the case for the excitation to the np\textsuperscript{(n+1)p} levels of Kr (n=4) and Xe (n=5) and to the np\textsuperscript{(n+2)p} levels of Ar (n=3) [1,3] where the wave functions are dominated by configurations with a single value of \( j_c \).
Finally, figures 1(c) displays the results for the forbidden transitions. As compared to allowed transitions, these transitions have much smaller cross sections at higher energies though they have comparable magnitudes near threshold. Again, as discussed above, the cross sections for transitions between levels with the same core are larger than those where the core changes. These cross sections for all the forbidden transitions fall slightly faster than $1/E^3$ at higher energies. Note that the cross section for the transition from the $1s_1$ level to the $3p_8$ level with $J = 3$ is zero in our approximation from angular momentum coupling considerations.

We have fitted the ICS for the allowed transitions to the Bethe-Born form

$$ICS = \frac{1}{E} (c_0 + c_1 \ln(E)) a_0^2$$  \hspace{1cm} (1)$$

**Figure 1:** ICS for electron excitation of xenon: (a) the solid curve $1s_1 - 3p_2$, the dashed curve $1s_1-3p_4$, the dotted curve $1s_5-3p_2$, the dashed-dot curve $1s_5-3p_4$, and the dashed-double-dot curve $1s_5-3p_4$ transitions; (b) the solid curve $1s_3 - 3p_7$, the dashed curve $1s_3-3p_{10}$, the dotted curve $1s_5-3p_6$, the dashed-dot curve $1s_5-3p_7$, the dashed-double-dot curve $1s_5-3p_7$, the short-dashed curve $1s_5-3p_7$, the short-dotted curve $1s_5-3p_{10}$ transitions; (c) the solid curve $1s_3 - 3p_3$, the dashed curve $1s_3-3p_5$, the dotted curve $1s_3-3p_6$, the dashed-dot curve $1s_3-3p_7$, the dashed-double-dot curve $1s_3-3p_7$ transitions.

As well, we have found the cross sections for the forbidden transitions behave as

$$ICS = d_0 E^2 a_0^2$$  \hspace{1cm} (2)$$
at higher energies. The fitting constants $c_0$, $c_1$, $d_0$ and $d_1$ are given in table 3 and 4. The energy is in atomic unit. Since the excitation energies for transitions from the metastable states are less than 4 eV, these fittings can be utilized from 30 eV onwards. Note that the magnitude of $c_0$ and $d_0$ reflect whether or not there is a change in the core configuration as discussed above.

We have found that the cross sections for the forbidden transitions considered in Ar [3] behaved approximately as $E^{-3}$ as $E$ increases while in this case the power is slightly more negative at around -3.4.

4. Conclusions

We have used RDW method to study electron excitation of the lowest lying metastable states of xenon to the higher lying fine structure states of the $5p^57p$ manifold. We have given a detailed analysis of the individual fine-structure transitions which are reflected in our results. Our present theoretical study will supplement ongoing experimental work in this field and provides reliable data for use in plasma modeling studies.

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| Initial State | 1s5 | 1s3 |
|--------------|-----|-----|
| $3p_{10}$    | 0.74623 | 0.06233 | 4.89×10^{-3} | 5.49×10^{-4} |
| $3p_{9}$     | 0.36277 | 0.02033 | - | - |
| $3p_{8}$     | 2.33589 | 0.27723 | - | - |
| $3p_{7}$     | 0.07017 | 2.01×10^{-3} | 5.47×10^{-4} | 3.71×10^{-5} |
| $3p_{6}$     | 1.11031 | 0.12797 | - | - |
| $3p_{5}$     | 3.52×10^{-3} | 5.74×10^{-6} | 1.51459 | 0.11233 |
| $3p_{4}$     | 2.78×10^{-4} | 2.78×10^{-5} | - | - |
| $3p_{2}$     | 1.43×10^{-3} | 1.41×10^{-3} | 3.04581 | 0.37606 |

Table 3: Values of the constant $c_0$ and $c_1$ in equation (1) for the allowed transitions

| Atom Transitions | Xenon $d_0$ | $d_1$ |
|------------------|-------------|-------|
| $1s_3 - 3p_{9}$  | 4.32×10^{-6} | -3.41409 |
| $1s_3 - 3p_{8}$  | - | - |
| $1s_3 - 3p_{6}$  | 2.43×10^{-6} | -3.41560 |
| $1s_3 - 3p_{5}$  | 1.32×10^{-5} | -3.40019 |
| $1s_3 - 3p_{3}$  | 3.02×10^{-2} | -3.45539 |
| $1s_3 - 3p_{1}$  | - | - |
| $1s_5 - 3p_{5}$  | 2.99×10^{-3} | -3.45280 |

Table 4: Values of the constant $d_0$ and $d_1$ in equation (2) for the forbidden transitions