Excited-state $1s$-$2p$ absorption by aluminum ions with partially filled L shells

J. Abdallah, Jr., R. E. H. Clark, and J. M. Peek*
Los Alamos National Laboratory, P.O. Box 1663, Los Alamos, New Mexico 87545
(Received 1 April 1991)

The purpose of this paper is to quantify the role of initial configurations that have an electron beyond the L shell in $1s$-$2p$ absorption of aluminum ions. The study is done in the context of a recent x-ray transmission experiment and is based on a theoretical model that is in good agreement with the measurements. In addition, the method of Epstein will be used to study the temperature-dependent effect of excited states on the cross section for the individual ions. Results indicate that about 50% of the absorption is due to initial configurations that have an excited electron beyond the L shell, and the overall opacity of the $1s$-$2p$ manifold of transitions can be enhanced by these configurations at elevated temperatures for some ion species.

Recent advances [1,2] in computer hardware and software have made it possible to generate, store, and access the large volumes of atomic physics data needed to perform complicated spectral simulations. For local-thermodynamic-equilibrium (LTE) applications, these data include atomic energy levels corresponding to a given set of electron configurations and resolved transition arrays that are calculated to accurately represent the radiative transitions that occur between levels of the various configurations. These methods have been successfully used [3] to simulate the absorption properties of aluminum plasmas by reproducing, to a high degree of accuracy, experimental x-ray transmission measurements performed at the Rutherford Appleton Laboratory (RAL) [4] and at the NOVA laser facility [5]. The photon energy region examined by the experiments corresponds to the manifold of $1s$-$2p$ transitions for ions with partially filled L-shell ground states. The calculated atomic structure includes all $1s$-$2p$ transition arrays involving levels of initial configurations of the type $1s^2(2s2p)^w$ and $1s^2(2s2p)^{w-1}nl$. The symbol $(2s2p)^w$ defines all possible distributions of w electrons among the $2s$ and $2p$ shells. The values of principle quantum n were limited to $3 \le n \le 10$, and values of orbital angular momentum quantum number l were limited to $l \le 4$.

The purpose of the current paper is to present the relative importance of excited states from the $1s^2(2s2p)^w$ and $1s^2(2s2p)^{w-1}nl$ manifolds with regard to the RAL experiment. In addition, their effect on the total absorption is studied by calculating the correction factors of Epstein [6]. The factors are calculated for contributions due to absorption from only the $1s^2(2s2p)^w$ initial configurations and for contributions from all configurations listed in the preceding paragraph. The difference between these two correction factors is a measure of the importance of $n \ge 3$ satellite absorption.

Figure 1 shows the role of excited states with regard to the RAL experiment and an aluminum plasma at a temperature of 40 eV and a density of 0.0135 g/cm.[3] The dashed line was calculated including only the contribution of the ground configuration for each ion stage, while the solid line is the full spectral simulation. The figure shows that the ground configuration accounts for only a small fraction of the total absorption and structure. Note that each ion structure is labeled by the element corresponding to the number of bound electrons, and each structure is primarily due to initial states $1s^2(2s2p)^w$. Satellites corresponding to configurations of the type $1s^2(2s2p)^w nl$ from the ion of lower charge also contribute in the region because the $1s$-$2p$ transition energies of $1s^2(2s2p)^w nl$ approach those of $1s^2(2s2p)^w$ as n gets large.

An option was added to the LINES code [2] to compute absorption due to individual configurations. All fine-structure absorptions from an initial configuration are summed, and the results are reported as fractions of the total absorption for the given photon energy interval. Since the simulations are in good agreement with experi-

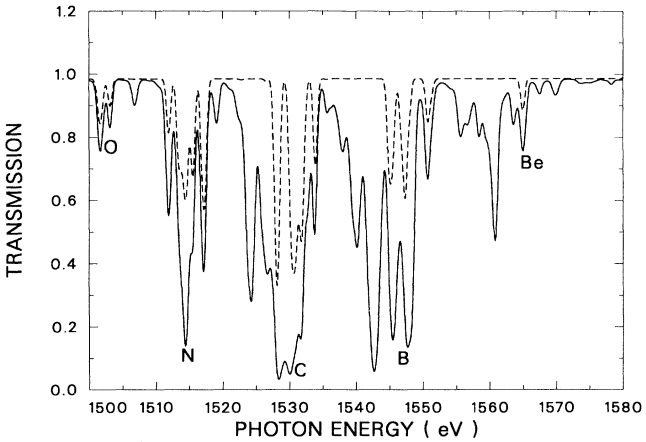

FIG. 1. Calculated aluminum x-ray transmission at a temperature of 40 eV and a density of 0.0135 g/cm^3, as a function of photon energy; the solid line includes all $1s^2(2s2p)^w$ and $1s^2(2s2p)^{w-1}nl$ initial levels while the dashed line includes only the contribution of the levels of the ground configuration.

TABLE I. The major contributors by ion and configuration to the total $1s$-$2p$ absorption calculated for the RAL plasma conditions.

Ion	Percent	Configuration	Percent
O	7.1		
N	28.7	$1s^2 2s^2 2p^3$	5.4
		$1s^2 2s^1 2p^4$	2.1
		$1s^2 2s^2 2p^2 3d^1$	1.1
		$1s^2 2s^1 2p^3 3d^1$	1.0
C	43.1	$1s^2 2s^2 2p^2$	12.9
		$1s^2 2s^1 2p^3$	11.3
		$1s^2 2s^1 2p^2 3p^1$	1.1
		$1s^2 2s^1 2p^2 3d^1$	1.5
B	18.8	$1s^2 2s^2 2p^1$	4.7
		$1s^2 2s^1 2p^2$	9.3
		$1s^2 2p^3$	1.8
Be	1.9	$1s^2 2s 2p$	1.1
	99.6		53.3

ment, a reasonable estimate of the absorption due to the various initial configurations should be obtained.

Table I provides a breakdown of the total absorption by an initial configuration for the plasma conditions discussed above. Initial configurations providing less than a 1% contribution are omitted from the table. Ground configurations account for about 23% of the absorption, and all $1s^2(2s2p)^w$ configurations account for 45%, leaving over 50% of the absorption due to configurations of the type $1s^2(2s2p)^w nl$. Most of these contribute less than 1% and therefore are spread over many configurations. Hence absorption by excited states plays a dominant role with respect to the RAL experiment.

Epstein [6] has recently discussed the effect of configurations of the type $1s^2(2s2p)^w$ on the $1s$-$2p$ absorption by chlorine ions. Useful formulas are provided for evaluating the temperature-dependent cross section due to states above the ground configuration for individual ions. The method is based on the total average absorption and assumes a Boltzmann factor for the relative population of states. The technique is useful for determining the effect of excited states on total absorption without interpreting complicated photon-energy-dependent line spectra. The correction factor f is given by the ratio of the total average absorption cross section σ to the cross section for absorption from the ground configuration σ_1, namely

$$f=\sigma/\sigma_1 , \tag{1}$$

where

$$\sigma=\frac{\sum_l g_l \sigma_l e^{-(E_l-E_1)/kT}}{\sum_l g_l e^{-(E_l-E_1)/kT}} \tag{2}$$

and

$$\sigma_1=\frac{\sum_m g_m \sigma_m e^{-(E_m-E_1)/kT}}{\sum_m g_m e^{-(E_m-E_1)/kT}} . \tag{3}$$

Here we have adapted Epstein's formula to apply to fine-structure levels. The parameter g_l is the statistical weight of level l, σ_l is the total integrated $1s$-$2p$ absorption cross section from initial level l, E_l is the energy of level l, T is the temperature, and k is the Boltzmann constant. The sum over l in Eq. (2) is performed over all excited levels, and the sum over m in Eq. (3) is performed only over levels of the ground configuration. The cross sections defined in Eq. (2) are independent of ionization balance and must be multiplied by the appropriate ion densities and summed to obtain total absorption.

Figure 2 shows a plot of f as a function of temperature for the various aluminum ions with from three to nine bound electrons. The calculations for Fig. 2 include only $1s^2(2s2p)^w$ initial levels, and hence look very similar to Epstein's results [6], which include the same configurations. The trend is a net lowering of the average cross section as the excited states become populated. This treatment may be adequate for describing the net decrease in $1s$-$2p$ absorption with increasing temperature due to excited configurations $1s^2(2s2p)^w$ in the narrow region near the main transitions from the ground state, provided influences of satellite lines from lower charge states can be neglected. However, it is not adequate for

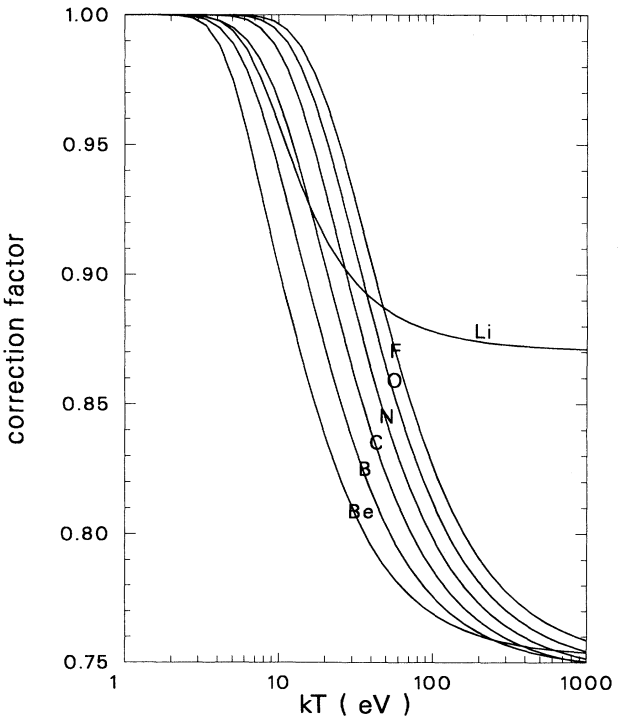

FIG. 2. Correction factors (dimensionless) as a function of temperature for the Li-like through F-like ions of aluminum including $1s^2(2s2p)^w$ initial levels only.

describing the average cross section for the complete manifold of $1s$-$2p$ transitions since higher excited states of the type $1s^2(2s2p)^{w-1}nl$ do play an important role even at moderate temperatures (see Table I).

Figure 3 is a plot of the correction factor f as a function of temperature for the appropriate ion stages using the more expanded set of excited levels corresponding to configurations of the type $1s^2(2s2p)^w$ and $1s^2(2s2p)^{w-1}nl$. The solid line includes all possible levels in the sum of Eq. (2), while the dashed lines limit the sum to initial levels below the ionization limit. In general, all the curves exhibit the same behavior. At low temperatures, the ground configuration dominates. As the temperature increases, the effect of the $1s^2(2s2p)^w$ excited levels is first observed by a lowering of the cross section. As the temperature is increased even further, f turns around and increases. This corresponds to an increase in population of the $1s^2(2s2p)^{w-1}nl$ levels. The correction factor is largest for the ions of lower charge (F and O) because of the initial limited vacancy in the $2p$ shell; as the temperature increases, the promotion of a $2p$ electron to an nl shell opens up the $2p$ shell and has a dramatic effect on f. As ion charge increases, the correction factors decrease. The Li-like ion has exceptional behavior because of its lack of statistical weight. The solid curves follow the dashed curves up to a particular temperature for each ion. The dashed curves have autoionizing initial levels left out of the sum in Eq. (2). These are mainly levels of $1s^2(2s2p)^{w-1}nl$, which have a more occupied $2p$ shell and a smaller cross section. Hence, the average cross section excluding these levels is greater than the cross section that includes them.

Figure 4 shows the calculated average cross section (solid line) of Eq. (2) and the ground-state cross section (dashed line) of Eq. (3) for each ion stage. The figure shows that the cross sections are proportional to the number of $2p$ vacancies, and that the opacity of the $1s$-$2p$ manifold of transitions is enhanced relative to the ground configuration for the F-, O-, N-, C-, and Li-like ions at temperatures proportional to M shell excitation energies. The cross sections may be used to obtain a rough estimate of the total $1s$-$2p$ absorption, independent of ion balance, over the photon energy range where these transitions occur.

Since the correction factors and average cross sections are essentially independent of the overall ionization balance, caution must be exercised when interpreting the 1-keV upper bound in Figs. 3 and 4. As temperature increases, the L shell becomes more ionized, and the contributions due to these ions become small. For example, under LTE conditions at a particle density of 10^{20} cm^{-3} and a temperature of 200 eV, L-shell ions account for less than 2% of the total population, mostly in the Li-like stage. At high densities there will be more L-shell population, and at lower densities there will be less. Therefore, some of the large differences at high temperature

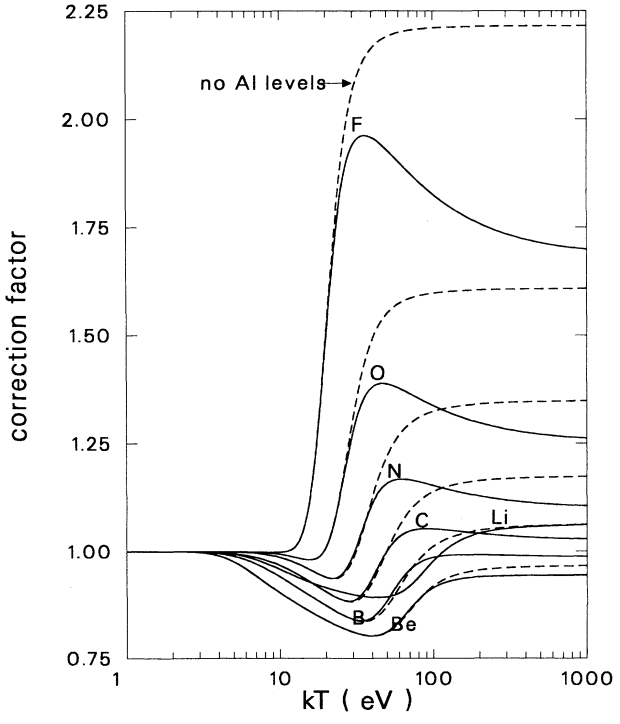

FIG. 3. Correction factors (dimensionless) as a function of temperature for the Li-like through F-like ions of aluminum; the solid line includes all possible initial levels of the configurations $1s^2(2s2p)^w$ and $1s^2(2s2p)^{w-1}nl$ while initial autoionizing levels were excluded in calculating the dashed line.

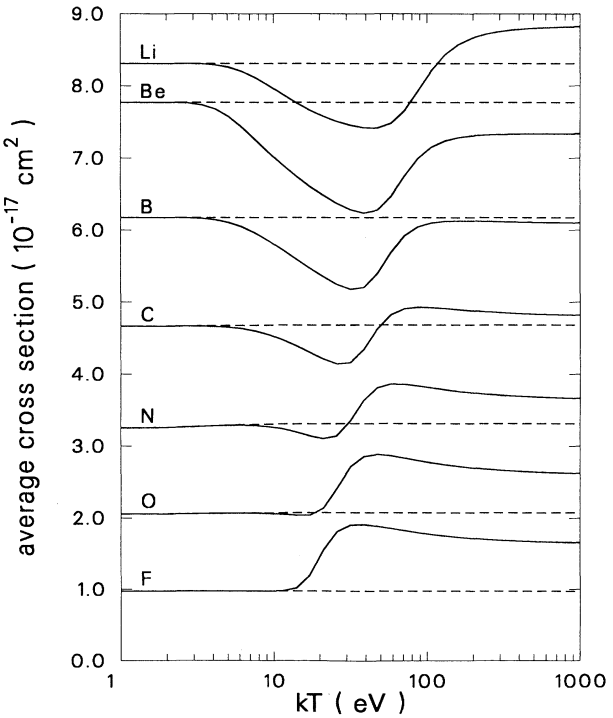

FIG. 4. Average cross section as a function of temperature for the Li-like through F-like ions of aluminum; the solid line corresponds to the total cross section and the dashed line corresponds to the cross section for the ground configuration only.

shown in Fig. 3 concerning autoionizing levels will have little effect in a LTE plasma.

With regard to the RAL experiment at $kT=40$ eV, the correction factors range from about 0.8 for the Be-like ion to about 1.4 for the O-like ion. The N- and O-like ions show cross-section enhancement, and the other ions show cross-section depletion with respect to their ground configurations. The treatment of autoionizing levels will have no effect on the spectral simulation for the higher charged ion species.

In conclusion, initial excited states of the type $1s^2(2s2p)^{w-1}nl$ account for about 50% of the $1s$-$2p$ total absorption observed in recent transmission experiments. The effect of these excited levels on the temperature-dependent average absorption cross section for individual ions was studied using a method presented by Epstein. Results show that the total absorption cross section can be enhanced relative to the ground cross section at certain temperatures for some ions.

This work was performed under the auspices of the U.S. Department of Energy.

---

*Present address: RFD 2, Green City, MO 63545.

[1] J. Abdallah, Jr., R. E. H. Clark, and R. D. Cowan, Los Alamos Manual No. LA-11436-I (1988) (unpublished).

[2] J. Abdallah, Jr. and R. E. H. Clark, Los Alamos Manual No. LA-11436-IV (1988) (unpublished).

[3] J. Abdallah, Jr. and R. E. H. Clark, J. Appl. Phys. **69**, 23 (1991).

[4] S. J. Davidson, J. M. Foster, C. C. Smith, K. A. Warburton, and S. J. Rose, Appl. Phys. Lett. **52**, 847 (1988).

[5] T. Perry (unpublished).

[6] R. Epstein, Phys. Rev. A **43**, 961 (1991).