Effects of Multiple Ionization on the K_α Spectrum of Aluminum in Intense Lithium Beam Experiments

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Abstract

The effect of multiple ionization on K_α spectra is investigated for aluminum targets irradiated by intense lithium beams. Multiple ionization cross sections have been calculated using a formulation incorporating single-electron ionization probability in the binomial distribution. In contrast to conventional binary-encounter approximation (BEA) theory, the single-electron ionization probabilities for each atomic shell have been calculated using a combination of modified plane-wave Born approximation (MPWBA) and an empirical effective interaction radius which is dependent on both the target ion and the projectile. Our calculations show that the effect of multiple inner-shell ionization on aluminum K_α spectra observed in intense lithium beam experiments is important. Multiple ionization effects becomes less important as the target ionization state increases. Nevertheless, even for highly ionized species up through Be-like Al multiple ionization effects can be significant and must be considered in the analysis of spectra obtained in intense Li beam-plasma interaction experiments.

1. Introduction

Atomic x-ray satellite spectroscopy has been widely used to diagnose plasma conditions in targets irradiated by intense ion beams (Nardi & Zinamon 1981, Bailey et al. 1990). For low- and medium-Z elements (atomic number Z $\leq$ 30), emission spectroscopy of K-shell lines is particularly useful. K_α emission lines result from transitions in which atomic states having a vacancy in the $1s$ shell decay to lower energy states as an electron from the $2p$ subshell fills this $1s$ vacancy. K_α satellite emission lines correspond to transitions with initial states having one hole in the K shell and n holes in the L shell. These satellite K_α lines are blue-shifted with respect to the principal K_α lines because of the reduced screening of the nucleus which results when there are fewer spectator electrons in the L shell. In the case of low- and medium-Z elements, the energy shift between consecutive satellites ($\Delta\lambda \sim 10^{-2}\lambda$), caused by introducing an additional hole in the L shell, is readily observable in present day laboratory plasma experiments.

K_α satellite emission spectra can be used as a temperature diagnostic for plasmas heated by intense ion beams because light-ion impact ionization of K-shell electrons populates autoionizing states, which then produce fluorescence K_α line emission. Since the K_α satellite lines from Ne-like to He-like ions exhibit detectable shifts to shorter wavelengths, K_α emission satellite spectra can provide a measure of the ionization distribution in a plasma, and from that, constraints on plasma conditions. However, it is important to note that measured K_α satellite emission spectra provide direct information on the autoionization state populations, as opposed to the bulk plasma (i.e., the low-lying energy states). The population states of the bulk plasma must be determined from ion beam-impact ionization cross sections. In this paper, we assess the importance of multiple ionization events (i.e., the simultaneous ejection of one or more L-shell electrons along with a K-shell electron) in intense Li beam experiments being carried out on Particle Beam Fusion Accelerator-II (PBFA-II) at Sandia National Laboratories.

In recent PBFA-II experiments, thin planar targets composed of Au, Al and plastic were irradiated with intense lithium beams (Bailey et al. 1993). A series of time-integrated Al K_α satellite spectra were recorded. In analyzing these data, it is critical to understand how multiple ionization can affect the spectra. The effect of multiple ionization on the K_α spectra may lead to inaccurate predictions of the ionization distributions of plasma if it is not properly accounted for. It is known (Richard et al. 1973) that the multiple inner-shell ionization of cold Al by alpha particle bombardment is significant. Hence, it is expected that at a minimum, multiple inner-shell ionization can have an important effect on the early time K_α line emission in the PBFA-II experiments when the Al is not highly ionized. On the other hand, as the plasma temperature increases the neutral and the low ionization stages of Al quickly disappear, and it is expected that multiple ionization effect should be less important for highly ionized Al because of the reduction of available number and the significant increase in binding energy of the L-shell electrons. Nevertheless, multiple ionization can still affect the line emission from satellites originating from higher ionization stages (MacFarlane et al. 1994).

In order to assess the importance of multiple ionization on the Al K_α spectra measured in recent PBFA-II Li beam experiments, we have performed a series of calculations to determine multiple ionization cross sections for Al ions up to Li-like. The relative importance of the multiple ionization processes are shown with intensities determined from ionization cross sections and fluorescence yields. Here we report on results showing the dependence of multiple ionization effects on (i) the Al target ionization state, and (ii) the Li beam energy.

2. Theoretical Models

Assuming that both the electrons and the shells are mutually independent, the cross section for simultaneous production of one K-shell and i $2s$-shell and j $2p$-shell vacancies can be expressed as (McGuire & Richard 1973)

$$\sigma^I_{K,ij} = N_K \int_0^{R_K} 2\pi b P_K(b) P_{ij}(b) db \tag{1}$$

where $P_K(b)$ and $P_{ij}(b)$ are the probabilities for single K-shell and multiple L-shell ionization, respectively. The sum $i + j = n$ is the total number of the L-shell vacancies. R_K is the distance at which $P_K(b)$ goes to zero. It has been shown (Hansteen & Hosebekk 1972, Watson et al. 1983) that a binomial distribution can be used to describe the probability of multiple ionizations in the target atoms. For the L-shell we have

$$P_{ij}(b) = C^i_2[P_{2s}(b)]^i[1 - P_{2s}(b)]^{2-i} C^j_6[P_{2p}(b)]^j[1 - P_{2p}(b)]^{6-j} \tag{2}$$

where $P_{2s}(b)$ and $P_{2p}(b)$ are the probabilities of single ionization from the $2s$ or $2p$ subshell, respectively, for an impact parameter b. The quantities C^n_m are binomial coefficients.

It is assumed that over the region $b \le R_K$, where $P_K(b)$ is nonzero, the probabilities $P_{2s}(b)$ and $P_{2p}(b)$ are constant. This is a reasonable assumption because $R_K << R_{2s}$, R_{2p}. Then we have

$$\begin{aligned} \sigma^I_{K,ij} &= N_K P_{ij}(0) \int_0^{R_K} 2\pi b P_K(b) db \\ &\simeq P_{ij}(0) \sigma^I_K \,. \end{aligned} \tag{3}$$

Thus, the multiple ionization cross sections for K1Lm (a configuration with 1 K-shell vacancy and m L-shell vacancies) is simply reduced to the product of the single K-shell ionization cross section and the zero impact parameter L-shell ionization probability.

The single subshell ionization cross sections can be calculated using a modified plane-wave Born approximation (MPWBA) which incorporates binding and Coulomb-deflection effects (Brandt & Lapicki 1981, Lapicki & Zander 1981). This method has been shown (Brandt & Lapicki 1981, Lapicki & Zander 1981, Chen et al. 1983) to produce much better results than the conventional plane-wave Born approximation (PWBA) for ion impact ionization cross sections. A comparison of the calculated cross sections of PWBA and MPWBA with the experimental data (Richard et al. 1973) for Al K-shell ionization by alpha particles is shown in Figure 1. Hartree-Fock wavefunctions were used in our calculations. It is clear the including binding and Coulomb deflection effects at low projectile energies ($\lesssim$ 3 MeV) leads to a significant improvement in the calculated cross sections. We used MPWBA in all our calculations.

The probability for single ionization at zero impact parameter of a given shell can be represented as (McGuire & Richard 1973)

$$P_i(0, \varepsilon_1) = \frac{\sigma_i(\varepsilon_1)/N_i}{2\pi R_i^2}, \tag{4}$$

where ε_1 is the energy of the projectile, N_i is the number of electrons in the ith shell of the target ion, and R_i is the effective interaction distance within which the projectile can interact with the electrons in the ith shell. Conventionally, R_i has been taken as the rms radius of the ith shell; i.e.,

$$R_i^2 = < r_i^2 > . \tag{5}$$

This procedure has been shown to produce good agreement with experimental data in the cases involving light projectiles such as protons and α particles (Kauffman et al. 1973). However, fundamental difficulties arise with the theory for higher-Z projectiles or very low Z targets. It is apparent that taking R_i to be independent of the characteristics of the projectile as shown in Eq. (5) is not adequate. Considering R_i as an effective interaction radius between target electrons and the projectile, it can be expected that this effective interaction radius will be larger as the nuclear charge of the projectile increases. From the point of view of polarization, R_i should be larger as $(Z_{\rm projectile}/Z_{\rm target})$ or $(v_i/v_{\rm projectile})$ increase. Here, v_i is the orbital velocity of the ith shell electrons. In accordance with our numerical tests, we have found that the following empirical expression for R_i gives much better overall agreement with experimental data for a wide range of projectile energies and projectile-target combinations:

$$R_i^2 = 4.69\sqrt{\frac{Z_{projectile}}{Z_{target}}}\sqrt{\frac{v_i}{v_1}} < r_i^2 > . \tag{6}$$

The resulting ionization probabilities calculated with the empirical R_i of Eq. (6) are listed in Table 1 and compared with the results of the binary-encounter approximation (BEA) (McGuire & Richard 1973) and experimental data (Kauffman et al. 1973). It is seen that the improvement due to the use of Eq. (6) is generally quite good. This is particularly true for more highly charged projectiles. We believe that the empirical model discussed above should provide reasonably accurate multiple ionization cross sections for low- to moderate-Z target plasmas irradiated by intense light ion beams.

3. Results and Discussion

With the empirical procedures discussed in Section 2 we have performed calculations for the recent Li beam-Al target experiments on PBFA-II (Bailey et al. 1993). The purpose of the calculations is to understand how multiple ionization effects have influenced the observed K_α spectra. The energy of the lithium beam is typically in the range of 8 - 10 MeV. The relative intensities of different satellite lines in the figures shown in this section are weighted by the ionization cross sections and the corresponding fluoresence yields, namely

$$I(Lm : a \rightarrow b) = \sigma_{K1Lm}\,\omega(a \rightarrow b), \tag{7}$$

where the symbol Lm refers to electronic configurations with m vacancies in the L-shell. Our calculated average fluoresence yields, ω, for different configurations considered in the calculations are listed in Table 2.

The calculated relative intensities of K_α satellite lines for AlI and 9 MeV Li^{+3} projectiles are shown in Figure 2. From the figure it can be seen that multiple ionization processes lead to a very rich structure in the K_α spectrum, as satellites from KL0 to KL6 are seen. The double ionization process (KL1) dominates over other processes, and the single ionization process (KL0) is only the third important process in causing the x-ray emission. Similar effects are seen for Mg- and Na-like Al as shown in Figure 3.

For the Li beam-irradiated Al targets in recent PBFA-II experiments, lower ionization stages, such as Mg- and Na-like Al quickly disappear as the plasma temperature increases. The major contributions to the shorter wavelength satellites in the time-integrated K_α spectra come from emissions of more highly ionized species. It is expected that multiple ionization effects become less important as the ionization state of the Al target plasma increases because of the reduction of available number and the significant increase in binding energy of the L-shell electrons. To understand the role of multiple ionization to the K_α emissions of highly ionized Al, we have calculated a series of target ionization state dependent K_α satellite spectra. The calculated results are shown in Figure 4 and Figure 5. For Ne-like Al, double ionization is still the dominant event and the two strongest satellite lines are KL1 and KL0. Starting from F-like Al, the single ionization process becomes dominant, while the multiple ionization processes become less important as the ionization state increases. However, even for B-like ions (with ground electronic configuration $1s^2 2s^2 2p^1$) double and triple ionization processes can still make observable contributions to the K_α spectra (MacFarlane et al. 1994). This indicates that it is impossible to predicate the peak ionization state in the target plasma by just looking at the time-integrated K_α satellite spectrum. Accurate analyses of the spectra require detailed modelling of ion beam-impact ionization processes, in addition to the usual collisional and radiative processes which occur in high energy density laboratory plasmas.

The sensitivity of multiple ionization cross sections to the beam energy has also been studied. Results are shown in Figure 6. It is seen that for the energy range of interest the relative importance of the multiple ionization effect decreases as the beam energy increases. This phenomenon was also noted by Watson et al. (1983) for Ne targets.

4. Summary

We have reported on our analysis of the effects of multiple ionization on Al K_α satellite spectra induced by Li beams. The empirical procedure we used has been shown to provide reasonably accurate cross sections, and represents a significant improvement over the conventional BEA model. Our calculated results show that the multiple ionization effect must be taken into account in analyzing the K_α satellite spectra of Al target plasmas created by intense Li beams. Our calculated multiple ionization cross sections have been applied to analyze K_α satellite spectra obtained in recent PBFA-II Li beam-plasma interaction experiments using a collisional-radiative equilibrium (CRE) model. These results are described elsewhere (MacFarlane et al. 1994).

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Table 1. Comparison of Calculated and Experimental 2p Shell Ionization Probability $P_{2p}(0)$ for Various Targets and Projectiles

Element	Experiment	This Calculation	BEA
(0.8 MeV Proton)			
Ca	0.012	0.012	0.013
Sc	0.011	0.011	0.011
Ti	0.0093	0.0093	0.0093
V	0.0054	0.0070	0.0079
Cr	0.0040	0.0061	0.0067
Mn	0.0028	0.0033	0.0057
(3.2 MeV α Particle)			
Al	0.13	0.12	0.15
Ca	0.044	0.039	0.054
Sc	0.038	0.033	0.044
Ti	0.031	0.027	0.037
V	0.025	0.023	0.030
Cr	0.018	0.019	0.027
Mn	0.010	0.016	0.023
(30 MeV O^{+5})			
Al	0.033	0.06	0.13
Ca	0.29	0.30	0.92
Sc	0.28	0.27	0.80
Ti	0.27	0.25	0.72
V	0.25	0.23	0.63
Cr	0.24	0.21	0.56
Mn	0.23	0.20	0.49

Table 2. Configuration-Averaged Fluorescence Yields for Al Ions

Configuration	Fluorescence Yield	Configuration	Fluorescence Yield
$1s^1 2s^2 2p^6 3s^2 3p^1$	0.043	$1s^1 2s^2 2p^6$	0.046
$1s^1 2s^2 2p^5 3s^2 3p^1$	0.046	$1s^1 2s^2 2p^5$	0.049
$1s^1 2s^1 2p^6 3s^2 3p^1$	0.081	$1s^1 2s^1 2p^6$	0.101
$1s^1 2s^2 2p^4 3s^2 3p^1$	0.048	$1s^1 2s^2 2p^4$	0.053
$1s^1 2s^1 2p^5 3s^2 3p^1$	0.098	$1s^1 2s^1 2p^5$	0.110
$1s^1 2p^6 3s^2 3p^1$	0.068	$1s^1 2p^6$	0.072
$1s^1 2s^2 2p^3 3s^2 3p^1$	0.052	$1s^1 2s^2 2p^3$	0.059
$1s^1 2s^1 2p^4 3s^2 3p^1$	0.116	$1s^1 2s^1 2p^4$	0.137
$1s^1 2p^5 3s^2 3p^1$	0.076	$1s^1 2p^5$	0.082
$1s^1 2s^2 2p^2 3s^2 3p^1$	0.060	$1s^1 2s^2 2p^2$	0.063
$1s^1 2s^1 2p^3 3s^2 3p^1$	0.220	$1s^1 2s^1 2p^3$	0.226
$1s^1 2p^4 3s^2 3p^1$	0.095	$1s^1 2p^4$	0.102
$1s^1 2s^2 2p^1 3s^2 3p^1$	0.051	$1s^1 2s^2 2p^1$	0.051
$1s^1 2s^1 2p^2 3s^2 3p^1$	0.310	$1s^1 2s^1 2p^2$	0.346
$1s^1 2p^3 3s^2 3p^1$	0.140	$1s^1 2p^3$	0.165
$1s^1 2s^1 2p^1 3s^2 3p^1$	0.350	$1s^1 2s^1 2p^1$	0.390
$1s^1 2p^2 3s^2 3p^1$	0.200	$1s^1 2p^2$	0.249

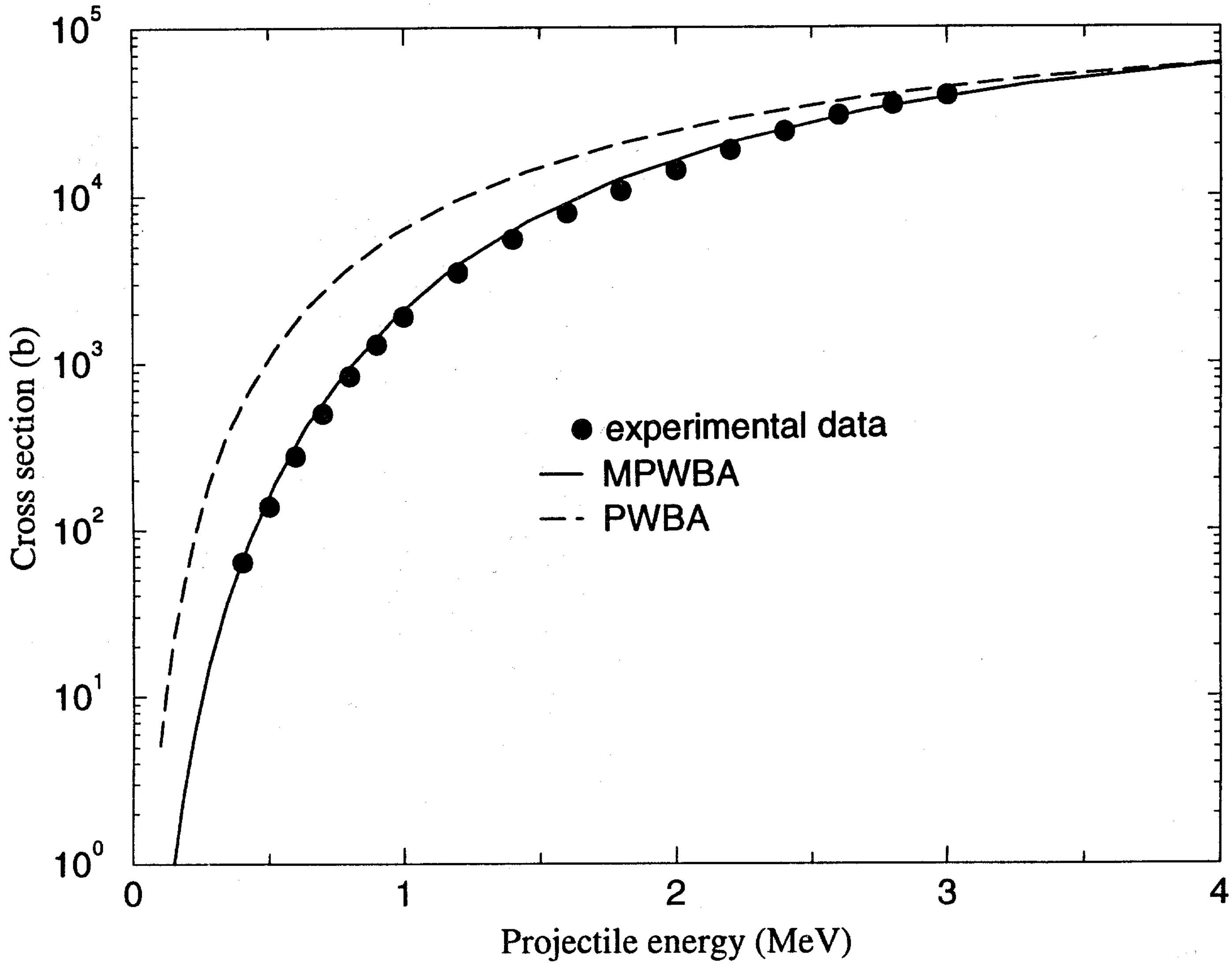

Figure 1. Al K-shell ionization cross sections by He^{+2} bombardment. A comparison of PWBA and MPWBA results with experimental data (Richard et al. 1973).

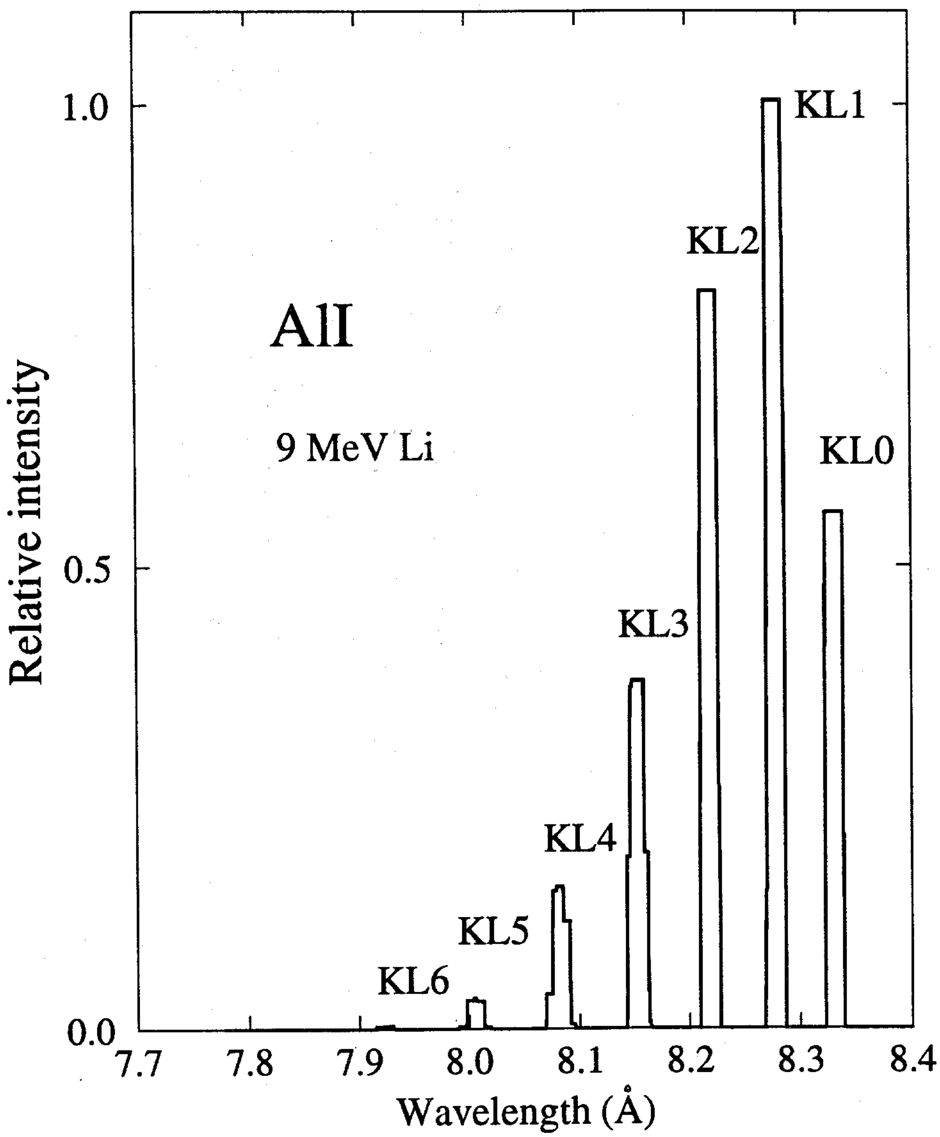

Figure 2. Computed relative intensities of Al K_α satellite lines for AlI bombarded by 9 MeV Li^{+3} ions.

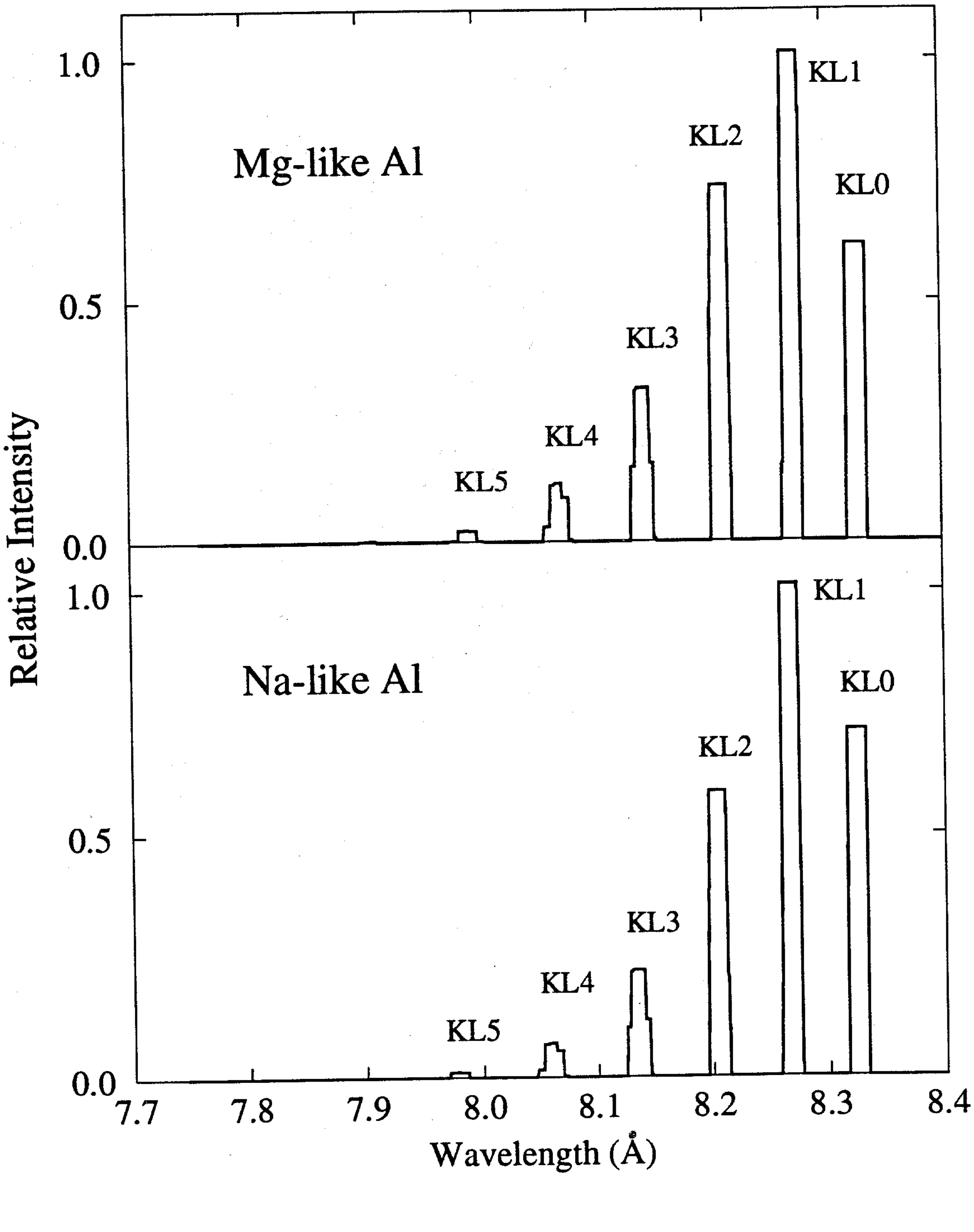

Figure 3. Computed Al K_α satellite lines for Mg- and Na-like Al ions by 9 MeV Li^{+3} bombardment.

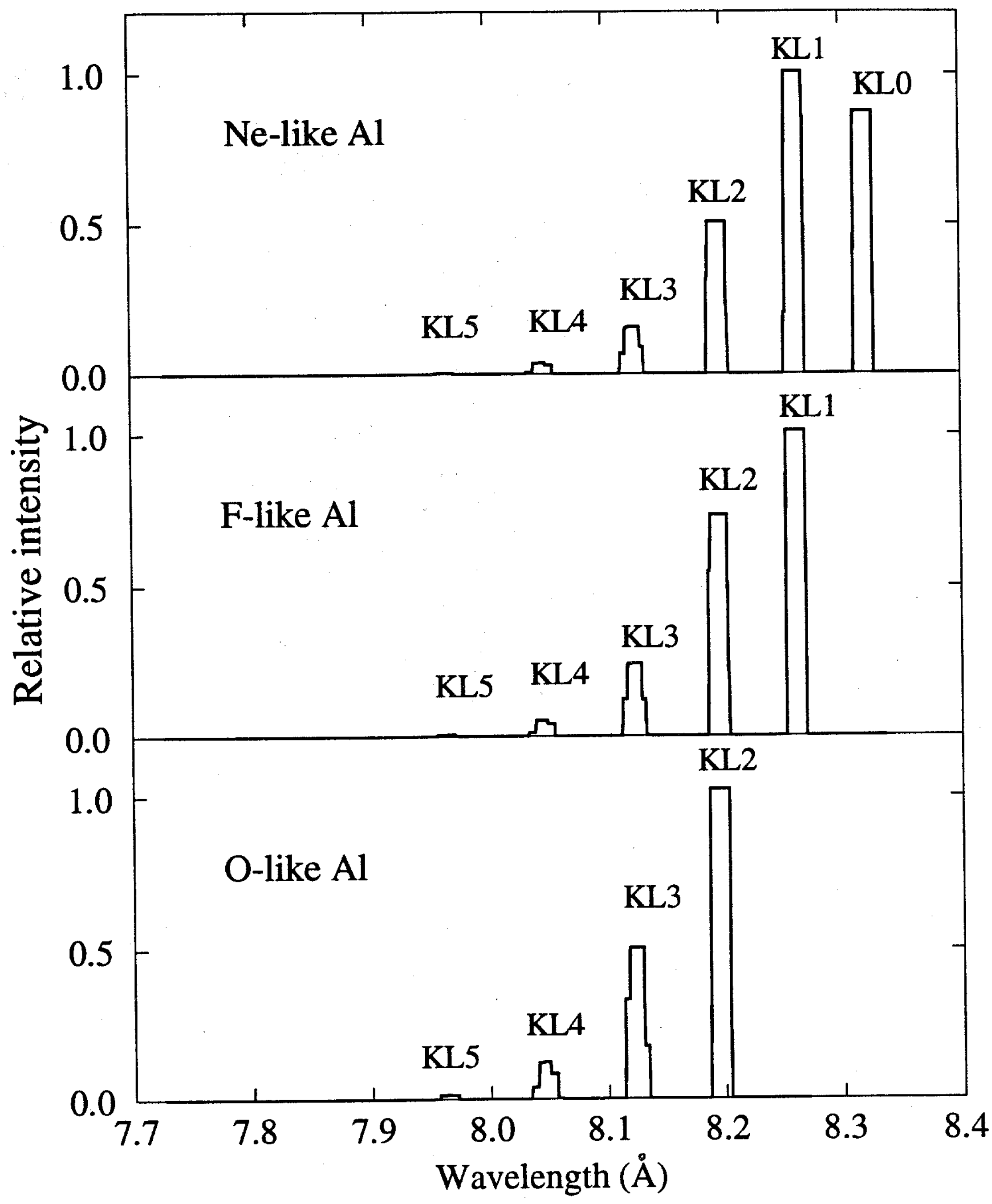

Figure 4. Computed Al K_α satellite lines for Ne-, F-, and O-like Al ions by 9 MeV Li^{+3} bombardment.

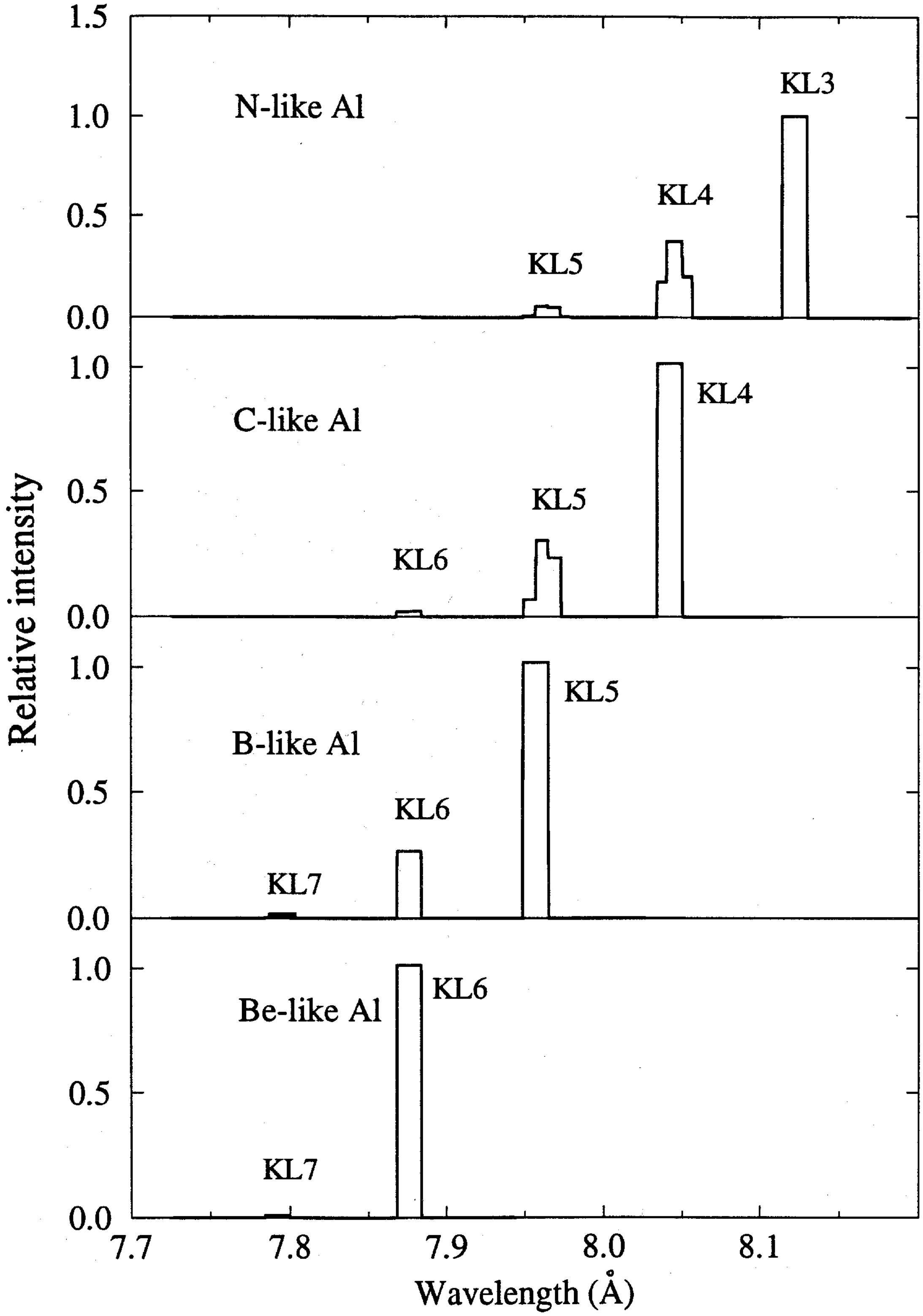

Figure 5. Computed Al K_α satellite lines for N-, C-, and B-like Al ions by 9 MeV Li^{+3} bombardment.

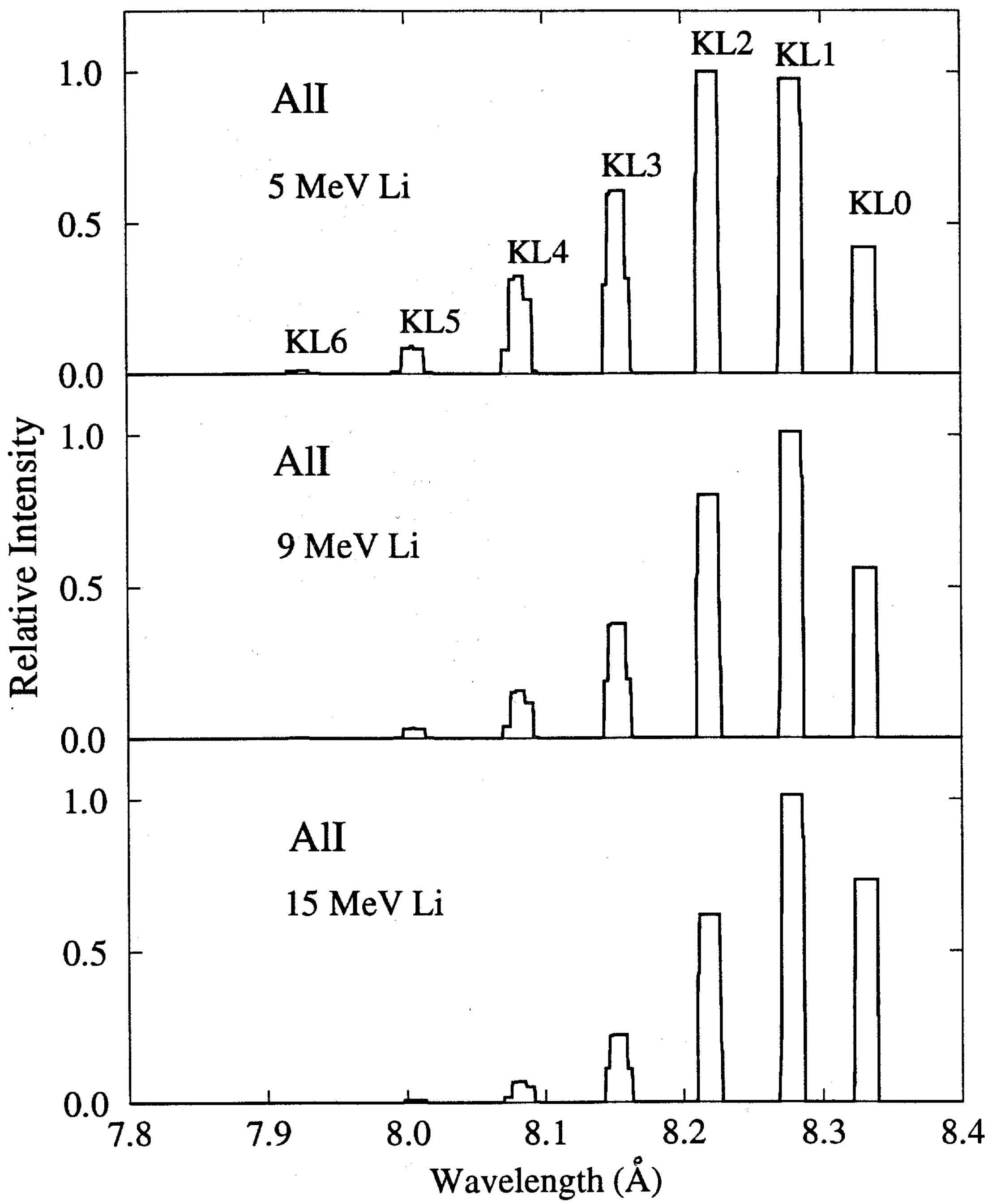

Figure 6. Computed Al K_α satellite lines for neutral Al and B-like Al ions by 5, 9, and 15 MeV Li^{+3} bombardment.