Thermal Ionization Effects on Inner-Shell Line Emission for Au Targets Heated by Intense Light Ion Beams

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Abstract

In order to deduce the experimental beam conditions from the observed x-ray line emission spectrum of high Z elements, atomic radiative data for transition energies and oscillator strengths, ion-atom impact ionization cross sections, Coster-Kronig yields, and fluorescence yield are needed. In this paper, we report on calculations to study the dependence of these atomic data on ionization stage. It has been found that proton impact ionization cross sections decrease slowly with increasing ionization stage, and the fluorescence yields have discrete jumps when the dominant Auger, Coster-Kronig transitions become energetically forbidden. Our study indicates that thermal ionization effects are not important for the dominant K, L and M line emissions for plasmas with $T_e \sim 10^2$ eV.

1. Introduction

The x-ray line emission from ion beam induced, inner-shell transitions of high Z elements can be used to diagnose experimental ion beam conditions. The measurement of the intensity ratio of two different emission lines allows one to determine the beam energy provided the x-ray production cross sections for the transitions of interest are known. Theoretically, the x-ray production cross sections can be deduced from ion impact ionization cross sections, radiative transition rates, Coster-Kronig yields and fluorescence yields. The methods for the calculations of these basic atomic data have been well developed and documented[1−4] and many atomic data tables are readily available.[5−8] To date, however, most of the calculations for these essential atomic properties have been performed only for neutral atoms. In present-day beam-target interaction experiments, the plasma is moderately ionized as it is heated to temperatures $\sim 10^1 - 10^2$ eV, with the dominant ions in high ionization stages. An important question is what is the dependence of these atomic properties on ionization stage, and under what conditions can the atomic data for neutral atoms be used reliably to analyze the emission spectrum of moderately ionized plasmas.

In this paper, we summarize results of our investigation to examine the ionization state dependence of proton impact ionization cross sections, Auger rates, Coster-Kronig yields, and fluorescence yields of K, L, and M shells for Au. Atomic radiative transition data were calculated using a relativistic multiconfiguration Dirac-Fock (MCDF) model. The calculations for ion impact ionization cross sections were made using a plane-wave Born approximation model with corrections for binding effect and Coulomb deflection[3]. For the calculations of Auger and Coster-Kronig transition rates, we used the LS coupling formalism of Burhop[2] with Hartree-Fock wavefunctions.

2. Calculations and Discussions

We have used Grant's MCDF program package[1] to calculate the atomic energy levels and radiative transition rates for the inner-shell emission lines of Au. This program enables one to carry out relativistic calculations with the inclusion of transverse (Breit) interaction and QED (self-energy, and vacuum polarization) corrections, which are thought to be essential to inner-shell transitions in heavy elements. The dominant radiative transitions for Au^{+0}, Au^{+19} and Au^{+62} with K, L, and M shell vacancies are listed in Table I along with the corresponding radiative transition rates. It can be seen that the radiative transition rates change only a few percent from neutral atom to very highly ionized ions. This is because the modifications of inner-shell orbitals by the thermal ionization of outer shell electrons is very small.

Table I

Dominant Radiative Transition Rates for Au Ions with K, L, and M Vacancies

(in 10^{-4}/a.u., 1 a.u. $= 2.42 \times 10^{-17}$ s)

Transitions	Au^{+0}	Au^{+19}	Au^{+62}
$2p_{1/2}$ - $1s_{1/2}$	5257.4	5264.1	5293.9
$2p_{3/2}$ - $1s_{1/2}$	9086.8	9103.2	9158.5
$3d_{3/2}$ - $2p_{1/2}$	550.9	551.0	591.1
$3d_{5/2}$ - $2p_{3/2}$	466.2	468.7	504.6
$4f_{5/2}$ - $3d_{3/2}$	21.88	23.07	–
$4f_{7/2}$ - $3d_{5/2}$	19.87	19.91	–

Calculations for ion impact ionization cross sections have been made using a plane-wave Born approximation model with corrections for binding effect and Coulomb deflection[3]. A comparison of our calculated cross sections for L-subshells with the experimental data[9] is shown in Figure 1. Quite good agreement is achieved. In order to

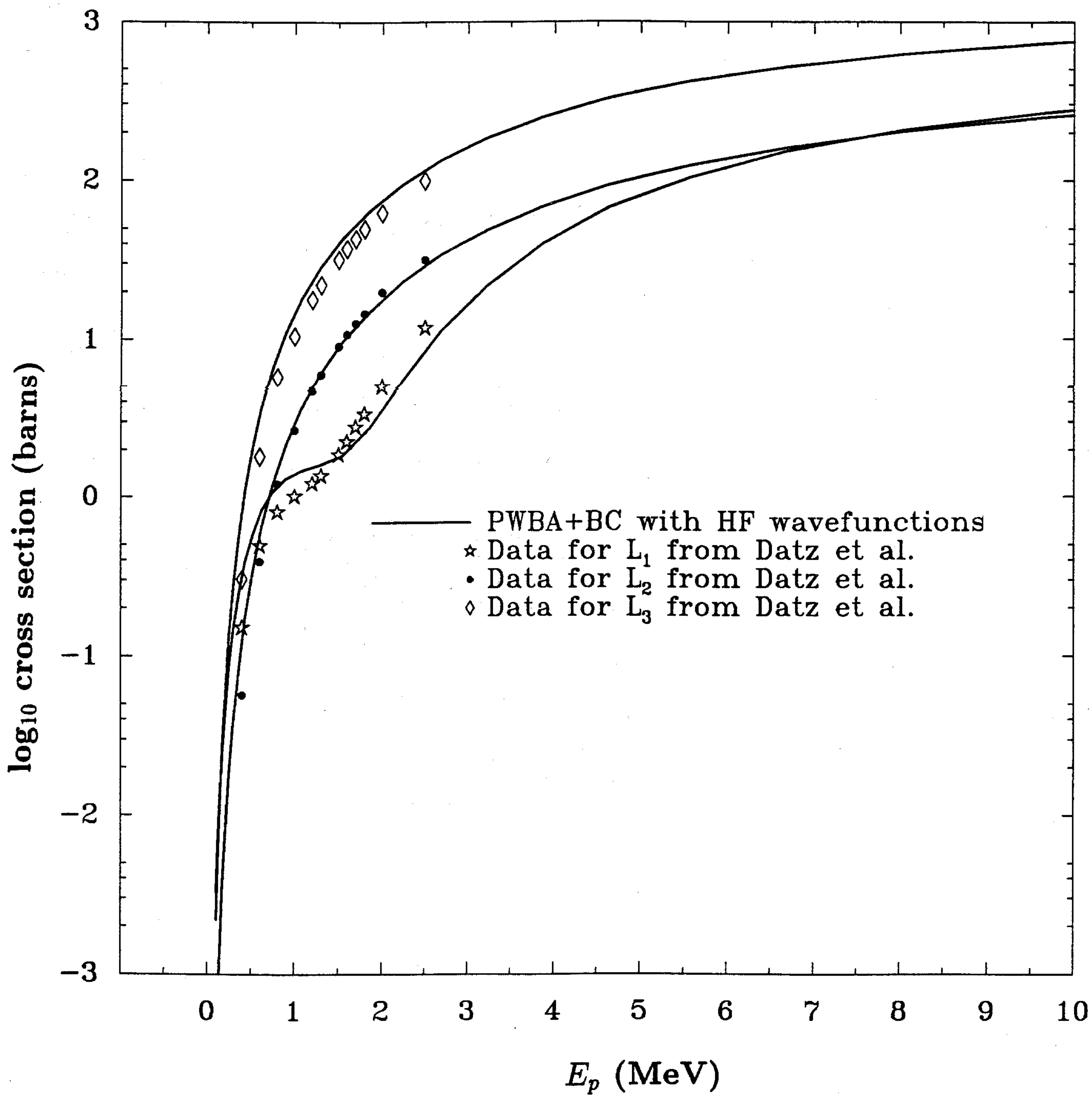

Figure 1. Proton impact ionization cross sections for L subshells of neutral Au.

examine the dependence of the cross sections on ionization states, we have done a series of calculations for ions ranging from Au^{+0} to Au^{+29}. The results for the M_5-subshell are presented in Figure 2. It can be seen that the proton impact ionization cross section is reduced by about a factor of 2 from Au^{+0} to Au^{+29}. The same situation happens to the other subshells; i.e., the ion impact ionization cross sections decrease slowly with increasing ionization stage.

The calculations of Auger and Coster-Kronig rates are based on the following formulations[10]:

$$\Gamma(nl_i, \epsilon l_j \rightarrow nl'_i, nl'_j) = 2\pi \sum | < i, j| \frac{1}{r_{12}} |i', j' > |^2 \tag{1}$$

and

$$< i, j| \frac{1}{r_{12}} |i', j' >= \sum_k x_k R^k(nl_i, \epsilon l_j; nl'_i, nl'_j|r), \tag{2}$$

where x_k is a coefficient related to the angular momentum coupling and $R^k(r)$ is the radial integral. It is easy to see that Auger and Coster-Kronig rates can only be related to the ionization state of ions through the radial integrals. Since the wavefunctions of inner shell electrons will not be sensitive to the ionization states, it can be expected that Auger and Coster-Kronig rates are not sensitive to the ionization states. In Table II we present the dominant Auger rates of $L_{2,3}$ vacancy for ions in several different ionization stages. The change of the Auger rates with ionization states is about ten percent so long as the transitions are energetically allowed.

The fluorescence yield for a specific transition $\omega(i \rightarrow j)$ is defined as follows[11]:

$$\omega(i \rightarrow j) = \frac{\gamma_R(i \rightarrow j)}{\Gamma_A + \Gamma_{CK} + \Gamma_R}, \tag{3}$$

where Γ_A, Γ_{CK} and Γ_R are the total Auger, total Coster-Kronig, and total radiative rate, respectively. We have seen that the radiative rate, Auger rate and Coster-Kronig rate for a specific inner-shell transition are not sensitive to the ionization stage. However, fluorescence yields are related to the total Auger and Coster-Kronig rates, and the

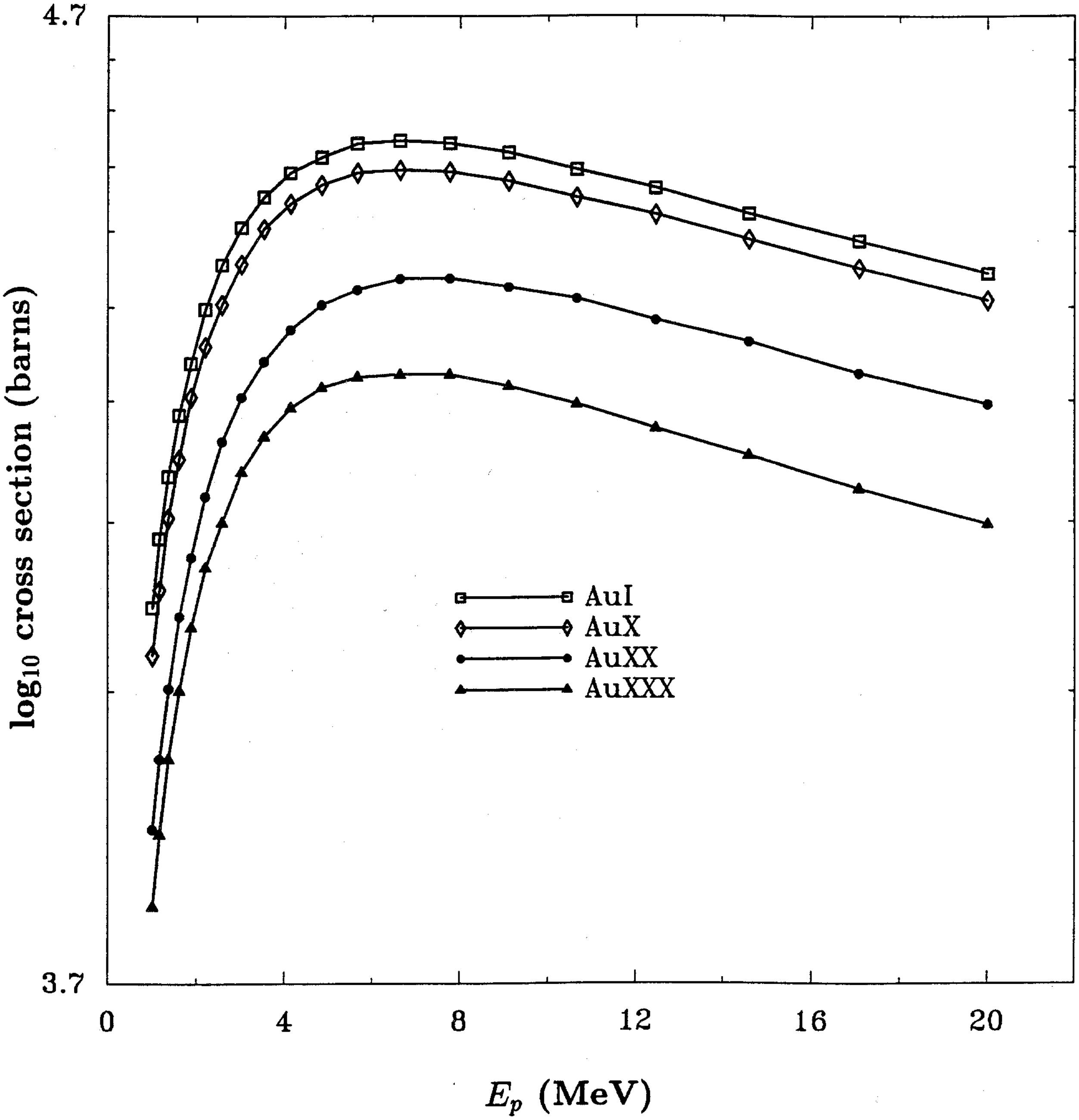

Figure 2. Calculated proton impact ionization cross sections for M_5 subshell of Au^{+0} to Au^{+29}.

Table II

L_{23} Auger Rates for Several Au Ions

(in 10^{-4}/a.u., 1 a.u. = 2.42×10^{-17} s)

Transitions	Au^{+0}	Au^{+1}	Au^{+17}	Au^{+33}	Au^{+53}	Au^{+61}
$L_{2,3} - M_{2,3}M_{2,3}$	129.7	130.1	128.3	133.5	137.9	139.1
$L_{2,3} - M_{2,3}M_{4,5}$	285.1	285.5	284.4	293.0	302.8	309.2
$L_{2,3} - M_{4,5}M_{4,5}$	478.0	478.9	471.5	488.9	502.4	509.9

Auger and Coster-Kronig transitions are subjected to the restriction of being energetically allowed. As the ionization stage increases, some of the Auger and Coster-Kronig transitions may become energetically forbidden, and hence cause a change in the fluorescence yield. Figure 3 shows how the fluorescence yields of K, L_1, and M_3 subshells for gold vary as a function of ionization stage. Also shown are the calculated results of Perkins[5] and McGuire[6–8]. Several features in the figure are of interest. First, the K shell fluorescence yield is basically unchanged from Au^{+0} to Au^{+19}. For L_1 and M_3 subshells, there are two discrete jumps. Point (1) is caused by the Coster-Kronig transition $L_1 - L_3M_4$ being energetically forbidden after Au^{+7}. Point (2) is caused by the Coster-Kronig transition $L_1 - L_3M_5$ being forbidden, point (3) is caused by the Coster-Kronig transition $M_3 - M_{4,5}N_{4,5}$ being forbidden, and point (4) is caused by the Coster-Kronig transition $M_1 - M_{4,5}N_{6,7}$ being forbidden. We have also made detailed calculations for other subshells L_2, L_3, M_1, M_2, M_4, and M_5. It has been found that the variation of fluorescence yield from Au^{+0} to Au^{+19} is less than twenty percent for these subshells.

Finally, a comparison of the energy-weighted ratio of L- and M-band for Au^{+0} and Au^{+15} is shown in Figure 4. It can be seen that the maximum difference of two sets of data is only about fifteen percent. This is because the change of fluorescence yields for the dominant radiative transitions $L_{2,3} - K$, $M_{4,5} - L_{2,3}$, and $N_{6,7} - M_{4,5}$ is small, and

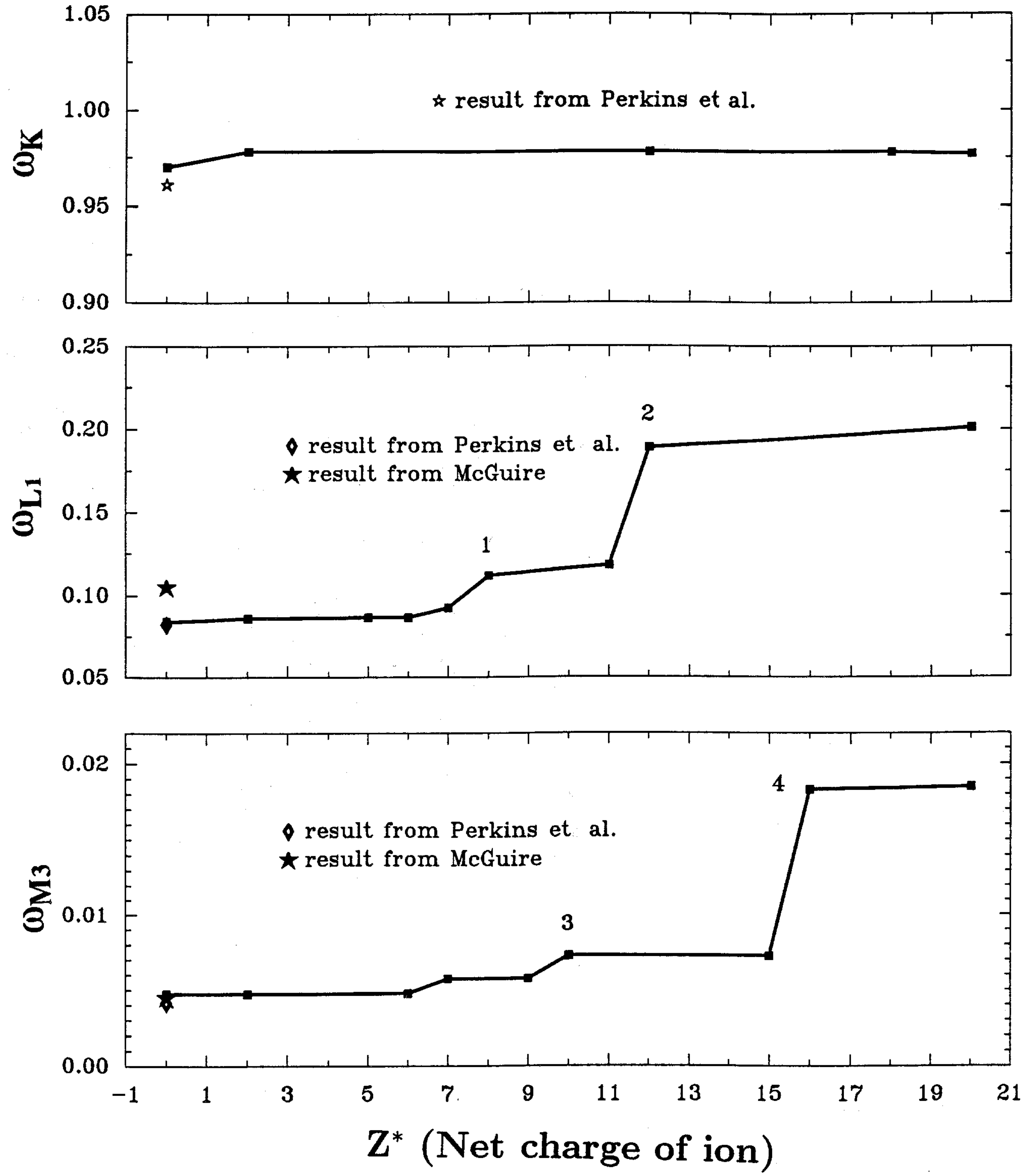

Figure 3. Fluorescence yields of different subshells as a function of ionization stage. Calculations for neutral Au from references 5-8 are also shown.

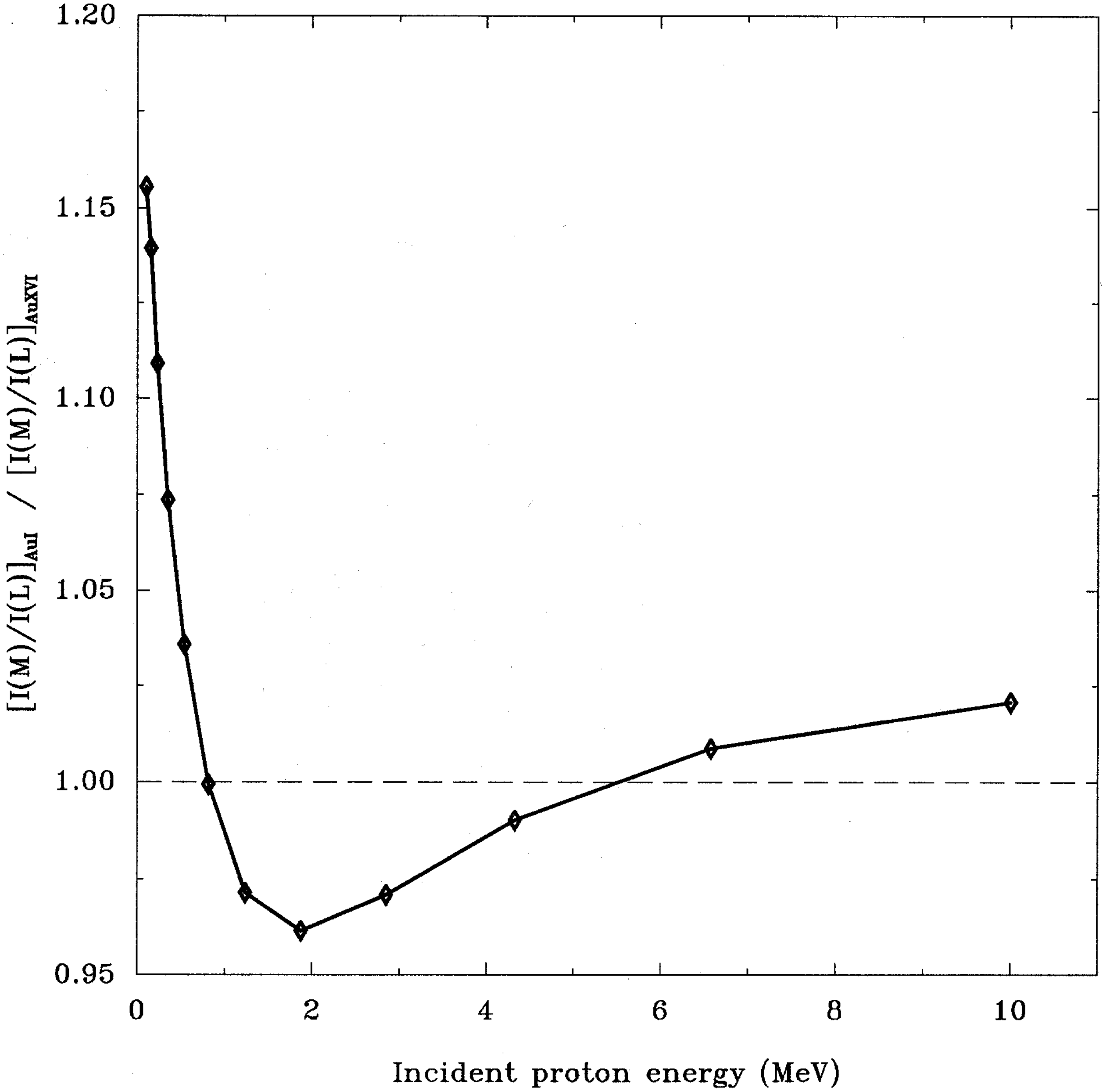

Figure 4. Comparison of the energy-weighted ratio of L- and M-band for Au^{+0} and Au^{+15}.

the decrease in proton impact ionization cross sections for L and M shells is about the same. Hence the net effect on the ratio of the two bands tends to be small.

3. Summary

We have studied the ionization state dependence of basic atomic data which are often used in deducing x-ray production cross sections by light-ion impact. The conclusions of this investigation are:

- The radiative rate, Auger rate and Coster-Kronig rate for a specific inner shell transition are not sensitive to the ionization stage.

- The fluorescence yield varies slowly with increasing ionization stage before the dominant Auger and Coster-Kronig transitions become energetically forbidden. Significant changes in fluorescence yields occur only for L_1 and M_3 subshells which are related to relatively weak emission lines.

- The ion impact ionization cross sections decrease slowly as the ionization stage increases.

Under current experimental conditions for ion beam-target interaction experiments, the plasma temperature is expected to be $\sim 10^2$ eV. In this temperature regime, the average ionization degree of a Au plasma is about 10 to 15. Our calculations suggest that thermal ionization effects will not significantly affect x-ray production cross sections.

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