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SYSTEMATIC INVESTIGATION OF ELECTRON IMPACT EXCITATION-AUTOIONIZATION FROM THE GROUND STATE OF HIGHLY CHARGED GAI-LIKE IONS THROUGH ΔN=1 TRANSITIONS

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ABSTRACT

A systematic variation in the line intensity ratios of GaI-like and ZnI-like ions of rare earth elements has been recently observed in spectra emitted in a low density, high temperature Tokamak plasma. This variation is shown to be correlated with the gradual opening of autoionizing channels through inner-shell excited configurations of the GaI-like charge-state. These channels enhance the indirect ionization rate of GaI-like ions through excitation-autoionization (EA), effecting the ionization balance and temperatures of greatest abundance. We present a systematic investigation of EA and direct impact ionization (DI) in the GaI-like isoelectronic sequence from Mo (Z=42) to Dy (Z=66). As Z decreases from Dy to Pr (Z=59) the levels of the configuration $3d^94p4f$, which are excited from the ground state by strong dipole collisional transitions, gradually cross the first ionization limit of the ion and are responsible for this ionization enhancement. When Z decreases further an additional channel is opened through the configuration $3d^94p4d$.

1. Introduction

In this work we present a systematic investigation of ionization enhancement in the GaI-like sequence owing to the indirect combined process of collisional excitation followed by autoionization. Our motivation is the peculiar behavior of spectral lines of GaI-like rare earth elements observed in recent Tokamak experiments.[1] The gradual reduction in intensity of GaI-like lines relative to lines of adjacent charge-states, with decreasing Z between Dy and Pr, indicated that the GaI-like population was selectively reduced in the plasma.

Previous observations by several groups[2] of NaI-like ions have shown that excitation-autoionization (EA) may dominate direct impact ionization (DI) for this sequence, and strongly effect the ionization balance. Cowan and Mann[3] have suggested that indirect ionization may be important, in general, for ions whose ground configurations comprise a few electrons outside a closed shell since more electrons are then available for impact excitation than for DI. GaI-like ions, with the ground state $3d^{10}4s^24p$, fit the description, and were mentioned as candidates for this combined process.

2. Model For GaI-like Excitation-Autoionization

Since the 3d-4f collisional dipole excitation is particularly strong, EA can be important if the excited configuration $3d^94s^24p4f$ lies above the first ionization threshold. In Fig. 1 we have displayed the configuration average energy of configurations $3d^94s^24p4f$ and $3d^94s^24p4d$ along the isoelectronic sequence in units of the ionization potential, IP(Z). Indeed the 4p4f channel is available for $Z \leq 66$. The 4p4d channel is open as well for the lighter elements, and closes around Z=54. Of course the configurations have a finite energy

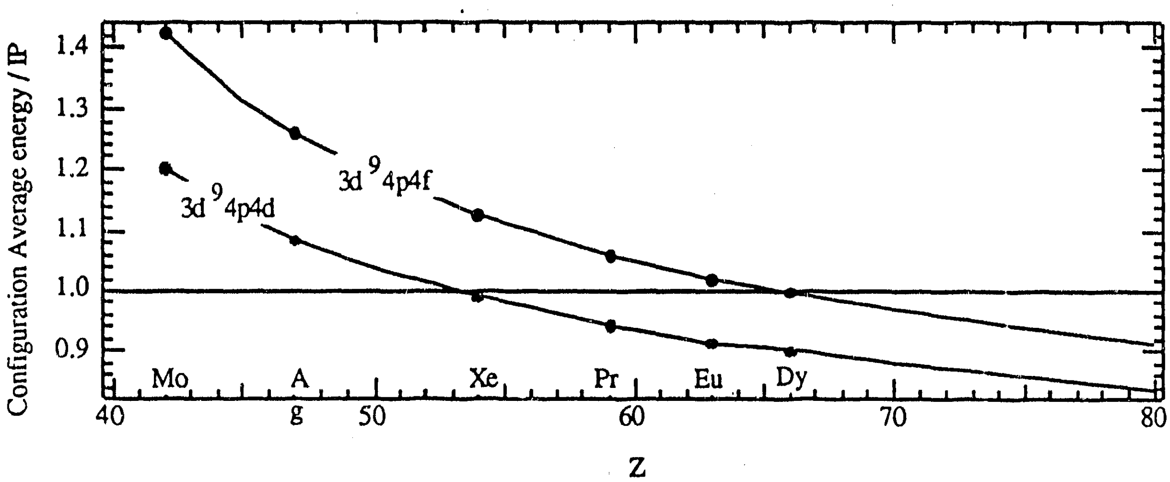

Fig. 1. Excitation-autoionization channels.

width, so that these channels are in fact partially open for a range of Z, and the configurations cross the ionization limit gradually.

To model the details of this combined process, including the situation where an excited configuration contains levels both above and below the ionization limit, requires a detailed level-by-level calculation. We have included in these calculations the relevant singly excited GaI-like configurations $3d^{10}4s^24p$, $3d^{10}4s^24d$, $3d^{10}4s^24f$, the inner-shell excited configurations $3d^94s^24p4f$, $3d^94s^24p4d$, and, to account for configuration interaction, $3d^94s^24p^2$ and $3d^94s^24d^2$. In the ZnI-like sequence, $3d^{10}4s^2$, $3d^{10}4s4p$ and $3d^{10}4s4d$ were included. Altogether, over 300 levels were included.

Level energies and radiative transition rates were calculated with the relativistic parametric potential model,[4] including CI. For collisional excitation and autoionization we have used the distorted wave approximation, and the factorization-interpolation technique.[5,6] Rate coefficients for DI were calculated in a modified plane wave Born approximation, using the free electron correction suggested by Vainshtein, *et al.*[7] All the necessary data was obtained for the six rare earth elements Mo, Ag, Xe, Pr, Eu and Dy.

Rates for EA were formed from rates of the elementary processes using the isolated-resonance approximation:

$$EA_{ik} \equiv \sum_j Q_{ij} \left[\frac{A^a_{jk}}{\sum_l \left[A^a_{jl} + A_{jl} \right]} \right] \tag{1}$$

where i denotes the levels of the initial GaI-like $3d^{10}4s^24p$ configuration, k denotes the final ZnI-like levels of the $3d^{10}4s^2$ or $3d^{10}4s4p$, Q_{ij} is the electron impact excitation rate to level j of the GaI-like inner shell excited $3d^94s^24p4d$ or $3d^94s^24p4f$ configurations, A^a_{jk} is the autoionization rate from level j to level k, and A_{jl} are the radiative decay rates to lower, singly excited, levels of the GaI-like ion. In our model we have included decays to the low lying configurations $3d^{10}4s^24p$,4d,4f. Detailed results will be presented elsewhere.[8]

3. Results

3.1 Z-Dependence

In Fig. 2 we present the results for EA from $3d^{10}4s^24p_{1/2}$, at an electron temperature equal to the first ionization energy. This rate is compared with DI as a function of Z. The ratio EA/DI is about 3 for Pr and about 0.2 for Dy. Similar behavior was obtained also for the $3d^{10}4s^24p_{3/2}$ level, except that, for this initial state, the ratio EA/DI drops only from about 3 at Pr to about 2 at Dy. However, in the Tokamak experiments,[1] the plasma density was only 4×10^{13} cm^{-3} and the $4p_{3/2}$ level was not populated owing to its magnetic dipole decay. Thus this channel was not active.

3.2 Density Diagnostics

The collisional excitation rate coefficient for the $4p_{1/2}$–$4p_{3/2}$ transition is $Q=1.14\times10^{-10}$ sec^{-1} cm^3, while the magnetic dipole transition rate is $M=2.8\times10^6$ sec^{-1}. At a density of 4×10^{13} cm^{-3} the excitation rate is three orders of magnitude smaller than the magnetic dipole transition rate. Thus, in the Tokamak, the population of the $4p_{3/2}$ level is roughly .002 that of the ground state. But at somewhat higher densities ($n_e>10^{16}$cm^{-3}), a density dependent EA rate is expected in Dy. A density dependent ionization rate has already been observed in some isoelectronic sequences, for example, BeI-like ions.[9] This should be the case not only for DyXXXVI, but also for the neighboring ions of the GaI-like isoelectronic sequence.

3.3 Temperature Dependence

The temperature dependance of ionization is shown for Pr in Fig. 3. The ratio EA/DI here is a decreasing function of T. This contrasts with the behavior of the NaI-like sequence investigated by Cowan and Mann.[3] They found a maximum in this ratio in the vicinity of the temperature of greatest abundance. The explanation for the difference can be found in Cowan's analysis. Using the semiempirical formulas of Seaton, Cowan showed that the ratio of the inner-shell excitation rate (EX) to the DI rate has the form

$$EX/DI \sim T^{-1}\exp(-\delta/T) \qquad (2)$$

This ratio has a maximum at T=δ, where δ is the difference in energy of the autoionizing configuration and the ionization threshold. In the NaI-like sequence δ is of the order of the ionization potential IP. But for GaI-like δ≈50 eV<<IP≈1000 eV and the point of maximum is far from the region of maximum abundance.

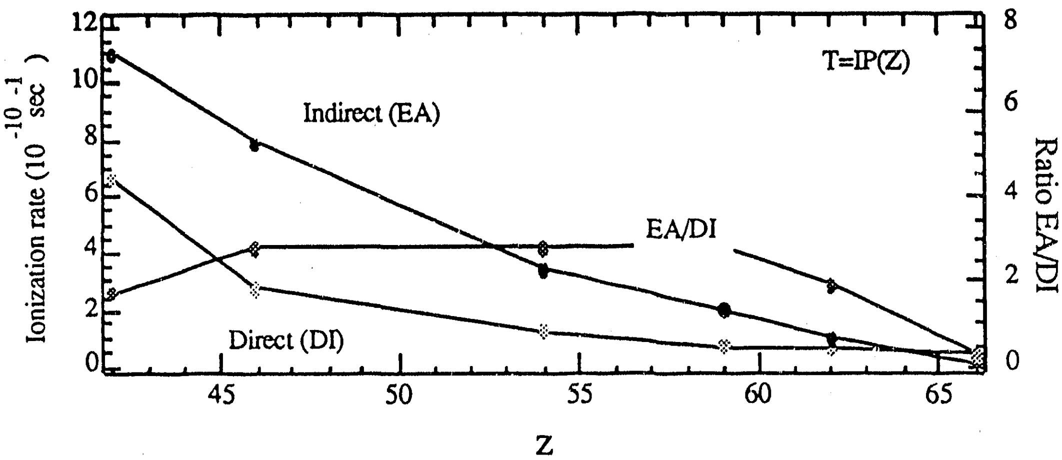

Fig. 2. Excitation-autoionization, direct impact ionization, and their ratio, as functions of Z.

3.4. Temperature Independent Change Along The Isoelectronic Sequence

To illustrate the behavior of the EA rate along the isoelectronic sequence in a temperature independent way, we construct an effective autoionization branching ratio for the 3d-4d and 3d-4f transitions, separately for the $4p_{1/2}$ and $4p_{3/2}$ initial levels. For each inner-shell excited configuration, C=$3d^94s^24p4d$ and $3d^94s^24p4f$, the branching ratio is the ratio of EA to total inner-shell excitation rate:

$$B^C \equiv \left[\frac{\sum_k EA^C_{ik}}{\sum_{j\in C} Q_{ij}}\right] \quad , \quad EA^C_{ik} \equiv \sum_{j\in C} Q_{ij}\left[\frac{A^a_{jk}}{\sum_l \left[A^a_{jl} + A_{jl}\right]}\right] \qquad (3)$$

These ratios are nearly independent of the electron temperature. In Table 1 these average branching ratios are listed as function of Z, at a temperature equal to the ionization energy of each ion, although it is very insensitive to this choice. As the energy of an excited level crosses from above the ionization energy to below, the branching ratio for autoionization falls. This occurs first for those levels excited from the $3d^{10}4s^24p_{1/2}$, then for those excited from the higher energy $3d^{10}4s^24p_{3/2}$. For the ions considered here, this effect is far more important than the decrease in branching ratio owing to increases in radiative decay rates with Z.

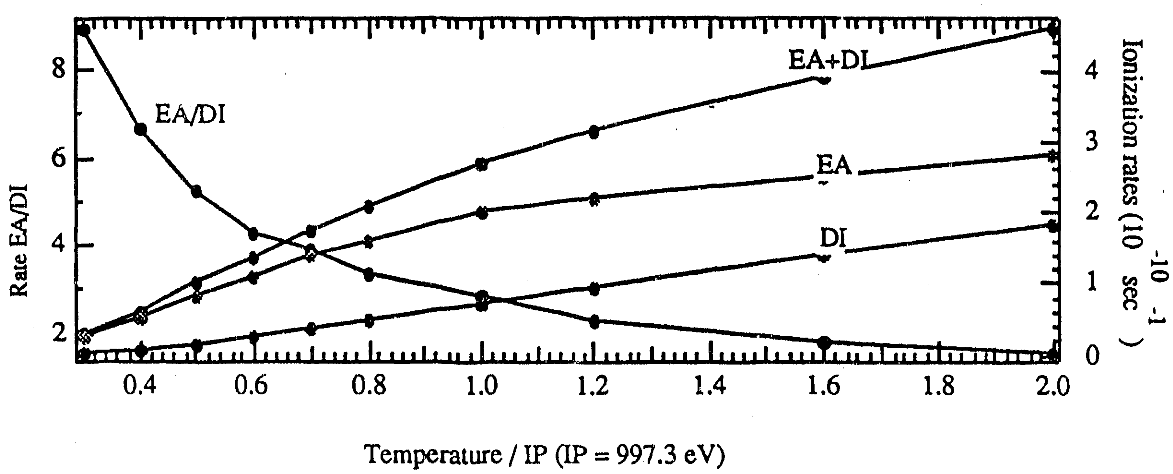

Fig. 3. Excitation-autoionization and direct ionization rates as functions of temperature for Pr XXIX.

4. Discussion

We have presented a detailed investigation of the behavior of EA and DI rates in the GaI-like isoelectronic sequence as a function of temperature and of Z. In particular we have found a dramatic change in the relative importance of these processes as Z changes from Pr to Dy. In order to estimate the relative abundance of these ions in the plasma, as reflected in the peculiar behavior of line intensities, one must solve the steady state ionization equilibrium equations taking into account direct and indirect ionization, as well as recombination processes for all the ionization stages. We have included in such a model the CuI-, ZnI-, GaI-, GeI- and AsI-like ionization stages. The rates for the various processes for these ionization stages were estimated from the semiempirical formulas of Seaton and Burgess. We solved for the relative abundance of these ions for various temperatures and found that including EA had two effects.

1) For Pr, as expected, EA reduces the ratio of GaI-like to ZnI=like ions. But because of the enhancement of the GaI-like due to EA from GeI-like ions, the reduction is by a factor of 1.5 only.
2) The temperature of greatest abundance for GaI-like Pr is reduced from 960 eV to 600 eV.

For Dy the GaI-like population is enhanced by EA from the GeI-like ion, and since this channel is closed for the GaI-like ion , the total effect of EA is an enhancement of the

GaI-like ion by 30%. The Temperature of greatest abundance of the GaI-like ion is also reduced here, but the change is small. In the Tokamak experiment,[1] the spectrum was emitted from the hot zone of the plasma, at T~1000 eV, where the two effects of EA worked to reduce the GaI-like for Pr, but not for Dy.

Table 1.

	$i=3d^{10}4s^24p_{1/2}$		$i=3d^{10}4s^2sp_{3/2}$	
	3d-4d	3d-4f	3d-4d	3d-4f
Mo XII	0.99	0.98	0.98	0.99
Ag XVII	0.96	0.95	0.89	0.96
Xe XXIV	0.12	0.88	0.68	0.87
Pr XXIX	0.00	0.69	0.00	0.70
Eu XXXIII	0.00	0.47	0.00	0.45
Dy XXXVI	0.00	0.05	0.00	0.37

5. Acknowledgements

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