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Precise and Accurate Calculations of Electronic Transitions in Heavy Atomic Ions Relevant to Extreme Ultra-Violet Light Sources

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Abstract

Precise and accurate calculations have been carried out for extreme ultra-violet optical transitions of atomic ions with atomic numbers ranging from 48 to 56. Intra N shell transitions of highly charged xenon and tin ions are investigated in detail in relation to the 13.5 nm band extreme ultra-violet light sources for the semiconductor technologies. The narrowing and the shift of the emission spectra of tin ions that were found by O'Sullivan and Faukner (Opt. Eng. **33**, 3978 (1994)) are discussed in detail. It has been pointed out that such the spectral narrowing and shift is common to the ions with atomic numbers that have been presently investigated for.

Keywords:

EUV, EUV light source, atomic transition, MCDF, configuration interaction

1. Introduction

In these decades, the 13.5 nm range extreme ultra-violet (EUV) light emissions of many electron atomic ions have become of interest in relation to the semiconductor lithography technologies. One of the best candidates for such the EUV light source are considered to be of the intra N shell (n = 4 shell) transitions or inter $N - O$ shell transitions of tin (Sn) or xenon (Xe) highly charged atomic ions.

It is normally indispensable to take into account the electron correlations if we are to evaluate the transition energies within the accuracy of a few electron volts, because the correlation energy of the atomic valence electrons falls in this range. We have to evaluate, on one hand, the intra N shell electron correlations precicely for excited states as well as the ground states. On the other hand, we have to notice that, in this type of the ions, especially of the Sn ions, a peculiar behavior in the emission spectra has been observed by O'Sullivan and Faukner [1]. They pointed out the narrowing and the shift of the 4f – 4d spectra as due to the interactions between $4p^6 4d^{N-1} 4f^1$ and $4p^5 4d^{N+1} 4f^0$ configurations, where N is an integer that runs from 1 to 9.

To gain a further insight of the effects, we have carried out careful MCDF calculations for $4d^N$ (N = 0 to 10) atomic ions with atomic number Z = 48 to 56, using GRASP (General purpose Relativistic Atomic Stracture Program)[2,3] and RATIP (Relativistic Atomic Transitions and Ionization Property)[4] family computer codes. We found, for example, that in the case of Sn^{12+}, the major peak positions of the 4s to 4f radial wavefunctions almost coincide, and, furthermore, that the differences of orbital energies between 4p and 4d orbitals, and 4d and 4f orbitals coincide within the range of 1%. The $4p^6 4d^1 4f^1$ and $4p^5 4d^3 4f^0$ configurations mix strongly, and the optical 4p – 4d and 4f – 4d transitions take place coherently, providing us with quite a peculiar EUV emission spectrum.

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2. Numerical calculation and results

To investigate the effect of intra-shell correlations, we have calculated the ground state energies of Xe^{8+} and Xe^{9+} ions with and without the $4d^2 - 4f^2$ correlations. The result is shown in Fig. 1. Although whole the $4f^2$ correlation energy exceeds 5 eV, the change in ionization potential of Xe^{8+} ion is as small as 1.5 eV. Because the energies of single electron excited states of Xe^{8+} ions will enter between the ground state energies of Xe^{8+} and Xe^{9+} ions and we may expect that their $4f^2$ correlation energies are more or less the same as of these ground state ions, we can disregard this correlation effect if we consider the value 1.5 eV is small. If not, we must consider the correlation effect properly.

To obtain the 4d – 4f transition energy of Xe^{8+} ions, we included the following configurations in the MCDF calculation, those are $4d^9 4f^1$, $4d^7 4f^3$, $4d^7 4f^1 5p^2$, $4d^9 5p^1$, $4d^7 5p^3$, $4d^7 4f^2 5p^1$, $4d^9 5f^1$, $4d^7 4f^2 5f^1$, $4d^9 6p^1$, $4d^7 4f^2 6p^1$. We have obtained 104.2 eV for the transition energy, which is 11.90 nm in transition wavelength. This value can be compared to the coresponding experimental data 12.01 nm [5]. To understand the origin of the differnce between the present calculation from the experimental data, we further included several configulations with higher lying f and p orbitals. However, the differnce of 0.11 nm could not be resolved.

As noted in a previous section, O'Sullivan and Faukner [1] have pointed out that there are strong interactions between $4p^6 4d^{N-1} 4f^1$ and $4p^5 4d^{N+1} 4f^0$ configurations in tin(Sn) multiply charged ions. To verify the effect, we made a calculation for Sn^{12+} ions. We illustrate the results in Fig.2. Due to the interference between the $4p^6 4d^2 - 4p^6 4d^1 4f^1$ and $4p^6 4d^2 - 4p^5 4d^3 4f^0$ transitions, we can observe a strong enhancement of the EUV emissions in 13.0 nm region, which provides us with the narrowing and shift in appearance of the emission spectra.

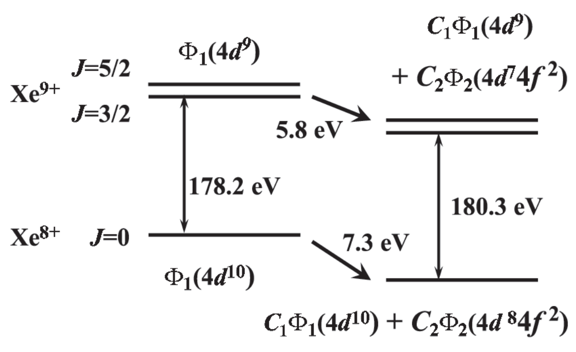

Fig. 1 Ground state intra-shell correlation energies of Xe^{8+} $4d^{10}$ of Xe^{9+} $4d^9$ and the changes in ionization potentials. The Xe^{8+} ground state energy falls off by 7.3 eV when we include the contribution of $4d^8$ $4f^2$ configuration. The Xe^{9+} ground state energy falls off by 5.8 eV when we include the contribution of $4d^7$ $4f^2$ configuration. The change in ionization potential is 1.5 eV.

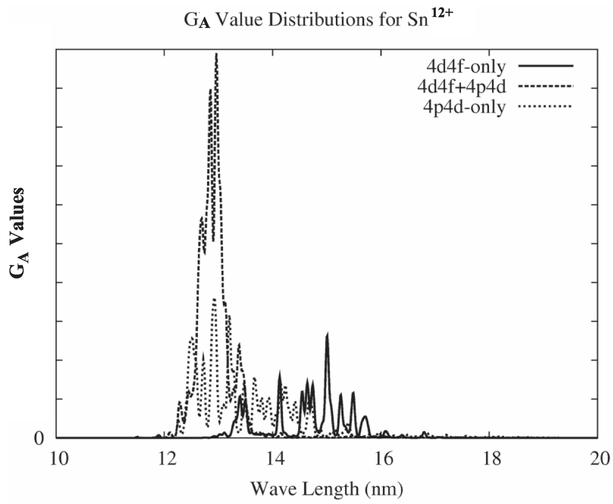

Fig. 2 The distribution of spontaneous emission rate G_A factors as function of EUV emission wavelength for 4d – 4f and 4p – 4d transitions in Sn^{12+} ions. The spectral distributions are convoluted with the artificial line width of 0.1 nm. The solid line represents the contibution of 4d – 4f transitions only. The dotted line represents the contibution of 4p – 4d transitions only. Whereas the dashed line includes both the contributions coherently.

Quite a similar effect has been obtained also for Xe ions, and further on for almost all the atomic ions with $Z = 48 - 56$.

3. Conclusion

The proper evaluation of the intra N shell electron-electron correlation effects is indispensable to obtain the energy of transitions with enough accuracy for the analysis fo EUV light source plasma. The dd – pf type configuration mixing is quite important to understand the peculiar spectral shape of EUV emission spectra of Sn ions. The strong dd – pf type configuration mixing are common to the atomic ions with $Z = 48 - 56$.

Acknowledgements

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