§34. Spectroscopic Measurements and Database Development for Highly Charged Rare Earth Elements

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The spectra of photoemissions due to the transitions between sub-shell levels in N-sub-shell open atomic ions are of interest for the strong influence from the interactions between the electronic state configurations with different constituent orbitals. Modifications in unresolved transition array (UTA) spectral profile has been pointed out^{1,2,3}, and this effect is advantageous to the development of practical extreme ultraviolet (EUV) light sources; the optical emission rates are strongly suppressed at large part of the transition energy positions, resulting in the spectral narrowing of the UTA spectra. The wavelengths of the 4*d* - 4*f* transitions are reported to be, for example, 7.9 nm for Nd (Z=60), 7.0 nm for Eu (Z=63) , and 6.8 nm for Gd (Z=64)⁴). The 4*d* - 4*f* transitions of Tb(Z=65) at 6.5 nm has been investigated theoretically by Sasaki et al⁵).

To study the EUV light emissions from highly charged heavy ions in connection to their atomic structures, it is quite effective to investigate in thin plasma conditions. We have proposed the use of the LHD plasmas for the spectral measurement of lanthanide elements. Up to the fiscal year 2014, we measured the emission spectra of a number of elements mainly from the lanthanide atoms. There was no LHD operation in the fiscal year 2015, and we could not perform the measurement scheduled to this year. In spite of this fact, we have presently covered almost the whole range of the atomic number in lanthanide atoms, say, for atoms with Z=58, 60, 62, 64, 65, 66, 67, 68, 69, 70, 71, and 72^{6,7)}. The present accumulation of the spectral data is now enabling our investigation on the Z-dependence of the spectral features in lanthanide elements. We are continuing the spectral analysis using the available data.

We compared those spectra to our elaborate atomic structure calculations based on a Multi-Configuration Dirac-Fock (MCDF) approximation. We employed the General purpose Relativistic Atomic Structure Program 92 (GRASP92)⁸ for the electronic structure, and the Relativistic Atomic Transition and Ionization Properties (RATIP) code⁹ for transition wavelengths and strengths. By using these programs, we can properly evaluate the electron correlations through the interactions between the relevant configuration state functions (CSF's) in a sophisticated manner. We have made the MCDF calculations for all the lanthanide atomic species for ions with the number of electrons from 27 to 59.

One of the most interesting features in the distribution of the spectral structures is the modifications of 4d-4f UTA. We firstly focused on these effects. In MCDF calculations, we optimize the individual single electron atomic orbitals

in Atomic State Function (ASF), which consists of the linear combination of CSF's, numerically by means of the self-consistent field (SCF) iterative procedure, and the coefficients of CSF's are simultaneously evaluated. We may find the optimum shapes of the single electron atomic orbitals that fit to the multi-configuration state under consideration. We can avoid the excessive expansion of ASF in terms of many CSF's which contain the variety of single electron orbitals; this feature gives us the chance to implement the realistic physical characteristics to the individual single electron orbitals. By using the minimal basis sets, we may obtain a physically plausible set of single electron atomic orbitals; we may discuss the physical property of the atomic ions in connection to the character of single electron atomic orbitals. In the present calculations, we included all the CSF's with one electron excitations to the sub-shell orbitals in the N-shell from the N-shell orbitals in the ground states. For instance, to calculate Gd^{26+} 1s²2s²2p⁶3s²3p⁶3d¹⁰4s²4p⁶4d² = [Ni]4s²4p⁶4d², we considered all the possible one electron excitations from $4s^24p^64d^2$ to 4d and 4f orbitals. We considered the configurations $4s^24p^64d4f$, $4s^24p^54d^3$, $4s^24p^54d^24f$, $4s4p^64d^3$. and $4s4p^{6}4d^{2}4f$, and all the possible ASF's are optimized simultaneously, which gives us a set of atomic orbitals that are common throughout the ASF's. By using the Relativistic Atomic Transition and Ionization Property (RATIP) package⁹⁾, we calculate wavelengths and the strengths of electric dipole (E1) transitions for all the possible combinations of the ASF's that are obtained by the MCDF procedure. In the case of Gd²⁶⁺ ions, for instance, we calculate the transitions to the ground states $4s^24p^64d^2$ - $4s^{2}4p^{6}4d4f$, and $4s^{2}4p^{6}4d^{2} - 4s^{2}4p^{5}4d^{3}$, as well as between the excited states $4s^24p^64d4f - 4s^24p^54d^24f$, $4s^24p^54d^3 - 4s^24p^54d^2f$, $4s^24p^54d^2f$, $4s^24p^5d^2f$, $4s^2d^2f$, $4s^2d$ $4s4p^{6}4d^{3}$, $4s^{2}4p^{5}4d^{2}4f - 4s4p^{6}4d^{2}4f$, $4s^{2}4p^{5}4d^{2}4f - 4s^{2}4p^{5}4d^{3}$, and $4s4p^{6}4d^{2}4f - 4s4p^{6}4d^{3}$.

Although we can consider the orbital relaxations in RATIP, we adopt the common basis orbital sets in both the states before and after the optical transitions. The non-orthogonality problem is not serious for E1 transitions in highly charged ions, and the accuracy of the calculations that are required is not as high as to urge us to adopt such sophisticated methods. And further on, by using the common basis orbitals, we can avoid the risk to face at large errors in the energy offset that come from the core electrons.

Detailed numerical calculations are now in progress.

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