



Electronic structure of multiplets and configuration interaction

Alexey A. Kornienko^{1*}, Elena Dunina¹, Liudmila Fomicheva²

¹ Vitebsk State Technological University, 210035, Vitebsk, Belarus

² Belarusian State University of Informatics and Radioelectronics, 220013, Minsk, Belarus

*a_kornienko@mail.ru

The hypothesis is formulated explaining why the configuration interaction sometimes strongly affects the deep-lying multiplets.

For the example of Nd^{3+} , Dy^{3+} , Ho^{3+} ions, the analysis of wave functions and the effect of configuration interaction on the intensity of absorption bands are considered. Attention is drawn to the fact that, because of the strong spin-orbit interaction, the wave functions of rare-earth ions are multicomponent superpositions of "pure" $^{2S+1}L_J$ multiplets with different values of S , L and the same values of the angular momentum J [1].

For this reason, the effect of configurational interaction depends not only on the energy gap to excited configurations, but also on the presence of high-energy $^{2S+1}L_J$ multiplets with different values of S , L and the same values of the angular momentum components. The presence of such components provides a strong influence of the configuration interaction even on the deep layers. Another consequence of the multicomponent composition of the wave functions is the formation of groups of strongly interrelated states. When the configuration interaction is not fully taken into account, the error in describing the oscillator strengths is distributed among all the states of the group, and the low overall accuracy of the description is not perceived as a contradiction of the theory. To confirm the proposed assumptions, the oscillator strengths of the absorption transitions of laser materials activated by Nd^{3+} , Dy^{3+} , Ho^{3+} ions have been described using the modified Judd-Ofelt theory.

References:

1. E. B. Dunina, L. A. Fomicheva, A. A. Kornienko, M. V. Grigoreva. *J. Appl. Spectroscopy*, 2018, Vol. 85, pp. 398–406.