Нанорозмірна фізика

EPR and luminescence spectrum interpretation by the modified crystal field theory. Prospects for nanosystem studies

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It is well known that the surface has an affect on the properties of nanosystems. In particular, a large number of atoms near the surface of nanoparticles, are situated in the highly distorted environment. The electron paramagnetic resonance (EPR) and optical spectroscopy both are the sensitive tools to obtain the unique information about the subsurface structure as well about the structure of the nanoparticles as a whole. For instance, paramagnetic ion which is embedded in the tested nanoparticles can act as a probe, which can vary the electron density distribution due to a change of the symmetry and the value of the crystal field distortions in the bulk and nanosized crystalline materials. As a rule, the crystal field theory is used to study the EPR and luminescence spectra. The mathematical and experimental complications arise for low-symmetry complexes and with a deficiency of crystallographic data. To avoid these difficulties, we propose a modified crystal field theory (MCFT) for the study of the EPR and luminescence spectra[*]. Undoubted advantage of this method is the ability to operate with a single parameter an effective nuclear charge of the impurity atom. This parameter can be determined from the experimental values of g-factors obtained from the EPR spectra. Thanks to simple parametrization, the MCFT gives the opportunity to explore coordination complexes with arbitrary symmetry and a set of ligands and to model different types of coordination complex distortions. The electronic spectra and *g*-factor values of an impurity ion can be simulated by arbitrary distortions of the ligand cage.

Above mentioned technique was applied to different compounds ($ZnAl_2O_4$, $LiGa_5O_8$, $ZnWO_4$), doped by Cu^{2+} ions. Moreover, this technique was tested on the luminescence spectra of the nanostructure carbon-nitride films, doped by the europium chloride CN_x : $EuCl_3$.Our calculations demonstrate the high sensitivity of the *g*-factor value also spectral lines to tiny distortions. Thus, the combination of EPR and luminescence techniques with the MCFT interpretation gives opportunity to study surface details of nanostructured compounds doped by impurity ions.

[*] *K. V. Lamonova*, *E. S.* Zhitlukhina, R. *Yu.* Babkin, *S. M.* Orel, *S. G. Ovchinnikov*, *Yu. G. Pashkevich* Intermediate-spin state of a 3d ion in the octahedral environment and generalization of the Tanabe-Sugano diagrams // J. Phys. Chem. A. – 2011. – V. **115**, № 46. – P. 13596 – 13604.