Nanoscale physics

Modeling electron spectra of nanoscale complexes formed by Cu ions on zirconia nanoparticles surface and bulk

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Modern progress of nanotechnology and microelectronics requires development of novel composite materials with predetermined properties. CuO-functionalized zirconia is the promising material for a wide spectrum of applications. Its structure and properties strongly depend on the synthesis conditions, in particular sintering temperatures. The main aim of our work was to explain theoretically an effect of the microenvironment on electron spectra of copper ions evident from experimental data obtained with the ESR technique.

ESR spectra of CuO-functionalized zirconia demonstrate nontrivial patterns. The spectrum is a superposition of two signals [1] showing the presence of paramagnetic Cu(II) centers with different surrounding ligands. Non-equivalence of ligands in axial and equatorial positions causes different degrees of tetragonal distortion of the octahedral crystal field.

Within the modified crystal-field approach proposed by us earlier [2], using the crystallographic data, we have analyzed distortions of coordination complexes CuL_6 (L = O, N) in both positions and studied numerically an effect of different types of the octahedral distortion on the electronic spectrum of Cu ions on zirconia surface. The calculations showed that in both complexes formed by Cu ions there are tetragonal distortions and a minimum of the adiabatic potential is formed by a tetragonal distortion of the octahedron.

The correlation between different types of distortion of the octahedral complex and the depth of minimum of the adiabatic potential has been found. The alteration of ESR spectra in different types of the adiabatic potential has been calculated and interpreted.

1. *Gorban O., Gorban S., Zarechnaya O., Kharchenko M., Konstantinova T.* Low temperature stages formation of interface composition systems Cu-Y-Zr-O, in book: Nanophysics, Nanophotonics, Surface Studies, and Applications, 2015.
2. *Lamonova K. V., Zhitlukhina E. S., Babkin R. Yu., Orel S. M., Ovchinnikov S. G., Pashkevich Yu. G.* Intermediate-spin state of a 3d ion in the octahedral environment and generalization of the Tanabe-Sugano diagrams // J. Phys. Chem. A.-2011.-**115.**-P. 13596-13604.