Vibrational Spectra of Co-Doped Hexagonal ZnO

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Zinc oxide (ZnO), due to the large direct band gap (Eg ~ 3.3 eV) at RT, large exciton binding energy (Ex ~ 60 meV) and strong excitonic emission, is widely used as a material for filters and detectors of UV radiation [1]. Doping with transition metal atoms opens another field of ZnO QDs applications. Diluted magnetic semiconductor QDs are the interesting materials for spintronics. Particularly, they can serve as memory cells and even as the logic elements for data processing due to their ability to store both electric charge and spin.

Despite ZnO is already well-studied and widely used in technology, the nature of its magnetic properties, which appear due to transition metal doping, is still far from clear understanding.

One of the most informative methods for studying such structural disorders is the Raman light scattering. In particular, micro-Raman studies are applicable even in the case of nanocrystals, while the X-ray analysis does not always allow to identify their structure distinctly. In contrast to undoped ZnO samples, Raman spectra of ZnO:Co samples demonstrate additional bands between LO and TO phonon modes, the intensity of which increases with the Co atoms' concentration.

In this work, vibrational density of states of 12.5% cobalt doped bulk hexagonal ZnO has been studied by the density functional theory method using generalized gradient approximation (GGA). We have considered various mutual positions of cobalt atoms in the structure including cases of single atoms and their complexes, as well as the possibility of cluster formation. It has been shown, that cobalt introducing into ZnO leads to appearing of additional vibrational modes with their frequencies dependent on the relative positions of the cobalt atoms. The magnetic and vibrational properties have been studied also of highly Co-doped ZnO samples, which are characterized by a high possibility of the metal clusters formation.

It has been found that two cobalt atoms forming Co-O-Co chain lead to a redistribution of vibrational density of states, and its maximum shifts to the region between TO and LO modes of ZnO. In addition, the cobalt clustering also may lead to appearing of additional modes with frequencies between TO and LO modes frequencies of ZnO, which are associated with the vibrations of Co-O-Co chains.

1. Ü. Özgür, Y. I. Alivov, C. Liu, A. Teke, M. A. Reshchikov, S. Doğan, V. Avrutin, S. J. Cho, H. Morkǫ, A comprehensive review of ZnO materials and devices // *J. Appl. Phys,* **98**, (2005), 1.