Magnetic Anisotropy Energy in Highly Co-Doped ZnO: Results of ab initio Studies

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The magnetic properties of the diluted magnetic semiconductors (DMS), caused by the substitution of cations by transition-metal ions, have become a subject of extensive studies in the past. The DMS have been recognized as the essential materials for semiconductor devices such as spin filters, spin polarizers or even spin transistors. After many years of studies devoted to the properties of cubic DMS crystals presently observed both theoretical and experimental effort has shifted to materials that exhibit the wurtzite-type crystal structure, grown on the basis of GaN or ZnO. The (Zn,Co)O is considered as the most probable DMS from the ZnO-based family for which the room temperature ferromagnetism could be both obtained and controlled. The present paper is devoted to the analysis of magnetic anisotropy energy (MAE) in (Zn,Co)O containing up to a few percent of Co.

There are several models of MAE in semiconductors. The discussion of models applicable for DMS can be found, e.g., in Ref. [1]. The challenge of magnetic anisotropy in (Zn,Co)O was analyzed recently in Ref. [2] where the authors calculated the dependence of MAE on the free-carrier concentration. In the present paper we have focused on different problem. The main challenge in the theoretical analysis corresponds to a dilemma as follows: does the observed anisotropy appear due to so called single ion anisotropy or is it related to the spin polarization of the host crystal atoms?

Density functional theory (DFT) calculations of MAE in (Zn,Co)O were performed using OpenMX package with fully relativistic pseudopotentials. The analysis of the band spin-orbit interaction and the magnetic ion's surrounding on MAE have been provided. We explicitly show that the magnetic anisotropy in (Zn,Co)O is of single ion anisotropy type, which means that MAE has been caused mainly by the cobalt ions. We show also that the wurtzite lattice parameters and the microscopic deformations of the Co ions nearest neighborhoods have significant influence on MAE value. As we believe, this could be of general importance for the quantitative analysis of MAE also in other, real crystals where, due to chemical disorder, such deformations have always been present.

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