Magnetic Anisotropy in GeMnTe – ab initio Calculations

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Recent magnetization and ferromagnetic resonance (FMR) measurements [1-4] show that in monocrystalline $Ge_{1-x}Mn_xTe$ layers grown on the BaF_2 (111) substrate with $x \leq 0.1$ the easy axis of magnetization is perpendicular to the layer. On the other hand, the usual in-plane easy axis due to dipolar interactions (shape anisotropy) is observed for polycrystalline and layered $Ge_{1-x}Mn_xTe$ with $x \geq 0.2$. X-ray analysis suggests that the change of direction of the easy axis is connected with the change of crystal structure: the increase of the manganese content leads to change of the crystal symmetry from rhombohedral to cubic.

Previous theoretical studies of anisotropy in semimagnetic semiconductors were based on the Zener model of ferromagnetism within effective–mass approach [5]. In the present work, first principles calculations of energy of magnetic anisotropy (EMA) in GeMnTe mixed crystals were performed using OpenMX package with fully relativistic pseudopotentials. The obtained results clearly indicate that EMA strongly depends on crystal structure, concentration of free holes and manganese content.

The discussion of microscopic origin of magnetic anisotropy was conducted. The main conclusion is that the magnetic anisotropy is caused by interplay between spin – orbit and Coulomb interactions. The results show that the change of spin direction of manganese ions results in spatial redistribution of the electron charge. The discussion includes the differences between conducting and insulating cases, in particular the range of spin polarization caused by manganese ions. Finally, we point out the important role of chemical disorder on the macroscopic magnetic anisotropy.

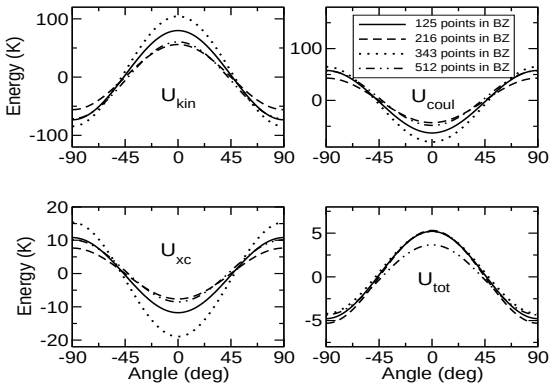

Fig. 1. Kinetic, Coulomb and exchange – correlation contributions to the total energy for the $2 \times 2 \times 2$ supercell containing one Mn ion as a function of angle between the spin direction of the ion and the [111] crystallographic direction. The hole concentration is $p = 5 \times 10^{21}\mathrm{cm}^{-3}$, the respective lines correspond to different discretizations of the Brillouin zone in the calculations.

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