Single ion magnetic anisotropy in disordered $Ge_{1-x}Mn_xTe$

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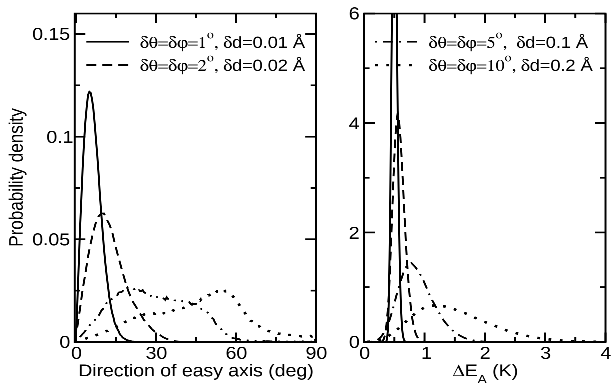
$Ge_{1-x}Mn_xTe$ mixed crystals atract a growing attention due to simultaneous presence of ferroelectric and ferromagnetic order (i.e., ferroicity). Unexpectedly, perpendicular anisotropy in thin layers was observed in magnetization and ferromagnetic resonance measurements. These experiments motivated our analysis of magnetic anisotropy energy (MAE) in $Ge_{1-x}Mn_xTe$ which lead to two important conclusions: 1) The main contribution to MAE comes not from the Mn ions, but from the polarized Ge and Te neighbors, 2) MAE strongly depends on hole concentration, crystal structure, and the local symmetry of Mn. In Ref. [1], the local symmetry of Mn was perfect rhombohedral. However, electron paramagnetic experiments show that the local symmetry of a magnetic ion determines its ground state splitting, and thus its magnetic anisotropy. Consequently, our analysis is extended here to single ion magnetic anisotropy of Mn in disordered $Ge_{1-x}Mn_xTe$ alloy.

There are two main causes of microscopic disorder in $Ge_{1-x}Mn_xTe$: 1) the different ionic radii of Ge and Mn, and random placements of Mn ions in the lattice, and 2) the very high concentration, of the order 10^{21} cm^{-3}, of Ge vacancies (which act as acceptors). The microscopic disorder is simulated by random changes ($\delta\theta_i$, $\delta\varphi_i$, δd_i, $i = 1, ..., 6$) of directions and lengths of bonds connecting the Mn ion with its six nearest neighbour Te ions. The applied method of calculations is nearly identical to the one used previously [2].



The influence of the disorder's level on magnetic properties is shown in the Figure. In the left panel we present probability distribution for the direction of easy axix of magnetization with respect to [111] crystallographic direction. In the right panel we show the probability distribution for ΔE_A, the difference between maximal and minimal values of anisotropy energies. In the paper the influence of disorder on magnetization is also discussed.

Our results clearly demonstrate that for realistic disorder in $Ge_{1-x}Mn_xTe$ crystals ($\delta\theta \sim \delta\varphi \sim 1^o$, $\delta d \sim 0.01$ Å) the single ion magnetic anizotropy is very weak, and therefore the observed MAE is mainly due to polarization of free carriers.

[1] A. Łusakowski and P. Bogusławski, *Acta Phys. Pol.* A **126**, 1177 (2014); A. Łusakowski, P. Bogusławski, and T. Story, arXiv:1502.01715v2 [cond-mat.mtrl-sci]
[2] A. Łusakowski and V. K. Dugaev, *Phys. Rev.* B **71** 014422 (2005)