Origin of uniaxial magnetic anisotropy in (Ga,Mn)As

M. Birowska[1], C. Śliwa[2], J. A. Majewski[1], and T. Dietl[1,2]

[1]Faculty of Physics, University of Warsaw, ul. Hoża 69, PL-00-681 Warszawa, Poland
[2]Institute of Physics, Polish Academy of Sciences, Al. Lotników 32/46, PL-02-668 Warszawa, Poland

We present the results of theoretical studies that shed light on the long standing and intriguing problem of uniaxial magnetic anisotropy energy (MAE) in (Ga,Mn)As [1,2]. We prove that the uniaxial MAE originates from the energetic preference of the [110] direction over the [1-10] one) for Mn ion pairs incorporated into the (001) surface of a GaAs substrate, leading to lowering of the crystallographic symmetry of the grown (Ga,Mn)As layers from cubic to C_{2v}, and in consequence to the uniaxial MAE. It is in accordance with the recent experimental and theoretical suggestions that the magnetism of the diluted magnetic semiconductors may be determined by the physical mechanisms governing the incorporation of the transition metals at semiconductor surfaces taking place during the non-equilibrium growth process [3,4].

Our findings are based on the *ab initio* calculations in the framework of the local density approximation to the density functional theory with relativistic pseudopotentials employed to account for the spin-orbit interaction non-perturbatively, and with effects of non-collinear magnetism included. Since the MAE is obtained from extremely small total energy differences, we carry calculations with extraordinarily high accuracy employing two numerical packages (SIESTA and QUANTUM ESPRESSO).

We have studied the energies of Mn pairs placed along the [110] and [1-10] directions of GaAs surfaces with various reconstruction patterns. It turns out that the [110] direction is energetically favorable. We have also performed calculations for all possible configurations of Mn pair substituted onto cationic sites of the 64 atom supercell. The configuration of the nearest neighbor Mn pair (implicating C_{2v} symmetry) has been energetically favorable by at least 0.025 eV/pair. This strongly suggests that the Mn pair configuration induced by the epitaxial growth can remain chemically stable in the bulk. Then, we have calculated MAE and determined six anisotropy constants for C_{2v} symmetry.

[1] D. Chiba, M. Sawicki, and Y.Nishitani *et al*., Nature Phys. **455**, 07318 (2008).
[2] M. Sawicki , K.Y. Wang, K. W. Edmonds *et al*., Phys. Rev. B **71**, 121302R (2005).
[3] A. Bonanni, A. Navarro-Quezada, *et al*., Phys. Rev. Lett. **101**, 135502 (2008).
[4] A. Navarro-Quezada, N. Gonzalez Szwacki *et al*., arXiv:1108.4901 (to be published in Phys. Rev. B).