Abstract

The scope of this thesis covers the *ab initio* study of the uniaxial magnetic anisotropy in the canonical example of dilute magnetic semiconductor DMS (Ga,Mn)As. The (Ga,Mn)As has become the focus of intense research over the past years. The spin-orbit mediated coupling of magnetic and semiconductor properties in this material gives rise to a large number of phenomena with a vast scope of possible applications in the field of spintronic devices. One of the intriguing phenomenon in this material is the presence of uniaxial magnetic anisotropy in structurally nominally cubic dilute magnetic semiconductor, which was not explained satisfactory before. The studies are done in the framework of the density functional theory (DFT), one of the most powerful techniques for a detailed understanding of real materials, and performed within the L(S)DA and L(S)DA+U computational schemes. The thesis has been divided into two main parts: (i) the surface-, and (ii) bulk calculations, relevant for the explanation of the mechanism of the uniaxial magnetic anisotropy in (Ga,Mn)As, and provides quantitative predictions of this phenomenon. In the first part of the thesis, the structural, electronic and magnetic properties of the isolated *Mn*-pairs onto the ideal (1×1) and reconstructed: (2×1), $\beta(2 \times 4)$, and $\beta 2(2 \times 4)$, *As*-terminated GaAs (001) surfaces are considered, with the *Mn* coverage corresponding to 1/8 of the layer. In all cases studied, we find that there exist the the nonhomogenous build-up orientations of the *Mn*-dimers onto the relevant surfaces, just in the moment of approaching the surface of the semiconductor. This non-random distribution of the *Mn*-ions at the surface is the physical origin of the symmetry breaking of the bulk GaAs crystal and consequently of the bulk uniaxial in-plane and out-of-plane magnetic anisotropies. In second part of the thesis, the magnitude of resulting magnetic anisotropies for the 6.25 % concentration of *Mn*-ions is discussed. Our results show that

the uniaxial magnetic anisotropy constants are order of magnitude greater then the experimental ones, indicating that the surplus of *Mn*-dimers residing in the preferred positions is only partial after the growth process. This suggests that it might be possible to control the strength of uniaxial anisotropy by changing the epitaxy conditions, particularly the growth rate and/or temperature. The influence of the various strains on the uniaxial magnetic anisotropy energy are also discussed. General trends for the applied biaxial or shear strains on anisotropy constants are consistent with the experimental data. The main achievement of the present thesis is that it points out, for the first time, plausible microscopic mechanism leading to the phenomenon of the magnetic anisotropy in (Ga,Mn)As.