Abstract:

The thesis presents a numerical study of magnetocrystalline anisotropies in dilute ferromagnetic semiconductors and transition metal systems intended to advance the current understanding of the microscopic origins of this relativistic effect and to contribute to the development of spintronic devices with new functionalities.

The major part of the work surveys magnetocrystalline anisotropies in (Ga,Mn)As epilayers and compares the calculations to available experimental data. Our model is based on an envelope function description of the valence band holes and a spin representation for their kinetic-exchange interaction with localised electrons on Mn^{2+} ions, treated in the mean-field approximation. For epilayers with growth induced lattice-matching strains we study in-plane to out-of-plane easy axis reorientations as a function of Mn local-moment concentration, hole concentration, and temperature. Next we focus on the competition of in-plane cubic and uniaxial anisotropies. We add an in-plane shear strain to the effective Hamiltonian in order to capture measured data in bare, unpatterned epilayers, and we provide microscopic justification for this approach. The model is then extended by an in-plane uniaxial strain and used to directly describe experiments with magnetisation direction controlled by strains due to postgrowth lithography or an attached piezo-electric stressor. We also study magnetisation switchings induced electrostatically in a field-effect transistor. The calculated easy axis directions and anisotropy fields are in semiquantitative agreement with experiment in a wide parameter range.

The second part of this work builds upon the experience gained in modelling magnetic anisotropies in (Ga,Mn)As and explores analogous spin-orbit coupling induced phenomena in ferromagnetic transition metal alloys. Our description of these systems is based on the tight-binding approximation with a realistic Slater-Koster parametrisation. We compare the predicted band structures, densities of states and magnetic anisotropy energies to ab-initio calculations first for elemental metals and then for CoPt and FePt ordered alloys. Qualitative agreement of ab-initio and tight-binding predictions is observed for the bimetallic structures. The applied formalism and the corresponding newly developed code allow for modelling magnetic anisotropies in systems with broken symmetry due to a finite multilayer structure, elastic strains or applied electric fields. Our work also provides practical basis for further research in this direction, in particular for studies of relativistic magnetotransport anisotropies by means of local Green's function formalism which is directly compatible with our tight-binding approach.