
Abstract

This dissertation presents a theoretical exploration of magnetic materials through a cycle of four articles published in peer-reviewed journals. Advanced computational methods were employed to investigate the structural, electronic, and magnetic properties of magnetic heterostructures, ferromagnetic ultra-thin films, antiferromagnets, and permanent magnets, providing insights into their behavior, modifications, and potential applications. The density functional theory within the implementation of the full-potential local-orbital code (FPLO) was applied to study the electronic structure of the materials. Additionally, the multislice method was employed to simulate transmission electron microscopy experiments, enabling the exploration of antiferromagnetic Bragg diffraction patterns. The results presented in the first article, covering the investigations of the magnetic properties in bcc iron-based heterostructures with an embedded atomic monolayer of transition metals, revealed agreement with the Slater-Pauling curve. Calculations also showed that Pt and W monolayers exhibit the strongest perpendicular magnetic anisotropy from all $3d$, $4d$, and $5d$ monolayers. The results in the second study, conducted in collaboration with the experimental group, identified a boundary-induced state at the Fe/MgAl₂O₄ interface, leading to the phase transition in ultra-thin iron films from body-centered cubic to body-centered tetragonal structure. Theoretical findings suggest that optimization of the substrate can enhance both the Fe film stability and the magnetocrystalline anisotropy energy. The third study employed a multislice method based on the paraxial Pauli equation, analyzing antiferromagnetic Bragg scattering in two antiferromagnetic materials NiO and LaMnAsO. The innovative computational approach of incorporating thermal effects for magnetic systems has allowed successfully reproduced experimental observations for NiO at room temperature. The study underlined experimental parameter optimization to detect antiferromagnetic Bragg scattering in materials consisting of heavier elements, which are increasing thermally diffused scattering. The fourth study examined the optimization of the magnetic properties of the CeFe₁₂ alloyed with transition metals and interstitial atoms. The results show, that alloying with the elements like Ti, Mn, and W enhances magnetocrystalline anisotropy energy, at the same time reducing the total magnetic moment, and leading to magnetic hardness sufficient to use selected materials as permanent magnets. Interstitial doping with light atoms like B, C, and N further tailored the magnetic properties of the selected alloys. Comparative studies with LaFe₁₂ revealed that Ce $4f$ electrons have a secondary impact on magnetocrystalline anisotropy energy value in the considered phases. The findings of the dissertation contribute to the design of advanced materials for spintronics and permanent magnet applications.

Keywords: density functional theory, multislice method, magnetic materials, thin films, ferromagnets, antiferromagnets, permanent magnets, magnetocrystalline anisotropy.