Abstract

The present habilitation thesis shows some of the most important results obtained by the author within two main research directions in the solid state physics: theoretical description of the spectroscopic properties (Compton scattering, positron annihilation and X-ray photoemission) and, respectively, band structure calculations, both used to describe the electronic and magnetic properties of solid state materials. The results described in this thesis have been obtained and published since December 2004 when the PhD degree (Magna cum Laude) has been obtained by the applicant at Ludwig-Maximilians University in Munich.

The main part of the research work enabling the present results has been developed within the research team from Babes-Bolyai University in Cluj-Napoca, where the applicant worked as postdoc (2005 - 2007) and scientific researcher (since 2007). Concerning the theoretical description of spectroscopic methods, the major scientific contribution described here is related to the development of novel calculation methods for Compton scattering and positron annihilation spectra in magnetic solids, based on the Korringa-Kohn-Rostoker (KKR) Green's function formalism. The theoretical description of the Compton profiles is a very useful tool for studying the electronic properties (i.e. momentum density or spin density localization). Some of the evidenced investigations are related to the study of the correlation effects on the magnetic Compton profiles (MCPs) of Ni and Fe. In particular, the role of the electronic correlations on the electronic structure of Ni has been evidenced by the direct connection between the 6 eV satellite feature of the Ni valence band and a broad contribution at the MCP from the energy window situated in the lower part of the valence band (Benea et al. [1]). On the other hand, focusing on the interplay between structural disorder and electron correlation in $Fe_{0.5}Ni_{0.5}$ and FeNi alloys, our studies demonstrate that the discrepancies between the experimental and theoretical MCP at low momentum can be diminished by adding the electron correlation within the theoretical description (Benea et al. [2]). Detailed studies reflecting the author's contribution in the Compton scattering studies are described in Chapter 1.

The momentum densities in solid state materials are subject of positron annihilation 2D-ACAR (Angular Correlation of electron-positron Annihilation Radiation) experiments. By the analysis of the electron-positron annihilation radiation recorded in 2D-ACAR experiment the electronic momentum density can be reconstructed. A main contribution of the author in this field has been the development of the formalism allowing for the theoretical description of the 2D-ACAR spectra. Using the combined theoretical and experimental approach on the 2D-ACAR spectra of 3d metals (Ni and V), their electronic momentum densities have been reconstructed and their special features have been interpreted [3, 4]. The inclusion of the electron correlation effects proved to be an important step in improvement of the Fermi surfaces description of 3d metals. The combined theoretical and experimental approach (in collaboration with the group of prof. C. Hugenschmidt from TU Munich) enables us to show the importance of an appropriate and accurate description of the momentum density in the case of 3d metals, allowing for interpretation of their special features, as can be seen in Chapter 2.

Photoemission spectroscopy, as a tool of investigation of electronic and magnetic properties of materials, has been used to study several systems, from metallic clusters embedded in $CaO\text{-}SiO_2\text{-}P_2O_5$ bioactive glasses to bulk magnetic materials, as $MnNi_{1-x}Sb_x$ and $Mn_{2-x}Co_xVAl$. Several electronic properties of these materials have been studied (degree of charge localization, the hybridization between the outer shells of neighbouring atoms or the dependence of the electronic structure on the size of specific metallic clusters) [5, 6, 7, 8]. A summary of these studies is presented in Chapter 3.

Electronic band structure calculations for investigation of the magnetic and electronic properties of solids have been performed for different type of systems: thin layers, clusters and bulk materials. Some of these studies, describing the theoretical and experimental investigations on the Fe hyperfine fields in Ti and Zr doped $Fe_{16}N_2$ [9] and the studies on the ground spin state of $Hf_{1-x}Ta_xFe_2$ [10, 11] are shown in Chapter 4. Also, theoretical and experimental investigations on the $HoFe_{2-x}Al_x$ and $Er_{1-x}Zr_xFe_2$ compounds with cubic C15 structure are discussed. The description of several properties of these materials, as magnetic ground state, magnetocaloric properties and the effect of different substitutions [12, 13] on their magnetizations and Curie temperatures is presented in first part of Chapter 4.

The most recent studies on half-metallic fully compensated ferrimagnets (HMFi) are related to the field of spintronics, being focused on development of new materials for spin transport, with lower stray fields and reduced energy consumption. The investigations performed on the half-metallic ferrimagnets $Mn_{2-x}Cu_xVAl$ and $Mn_2V_{1-x}Co_xVAl$ full Heusler alloys [8, 14, 15, 16] are presented in Chapter 5. Some of their properties are emphasized, which recommend them to be used in the future spintronic applications. The future plans for developing the author's professional activity are described at the end of this thesis in Chapter 6.