

# Spintronics

Claudia Felser • Gerhard H. Fecher  
Editors

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From Materials to Devices

 Springer

*Editors*

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# Foreword

Spintronics is a new field of science, developed over the past 20 years, that is focused on exploring the properties of materials in which spin-polarized currents play a key role, as well developing materials and devices for advanced nano-electronic applications. Spintronics materials have already found one important application in the form of highly sensitive magnetic field sensors in recording read heads for magnetic disk drives. The development of such “*spin-valve*” sensors was predicated on the discovery of the twin phenomena of giant magnetoresistance (GMR) and oscillatory interlayer magnetic coupling in magnetic multilayers formed from transition and noble metals in the early 1990s. More recently the same spin-engineering concepts in conjunction with the phenomenon of spin-dependent tunneling has allowed for the further development of even more sensitive recording read heads. Magnetic tunnel junction (MTJ) read heads have, since about 2007, have completely replaced sensors based on the phenomenon of GMR. Further advances in such recording read heads require new sensing materials that have a complex set of intertwined properties. Similarly, spintronics materials and phenomena, if suitably engineered, have the potential for novel solid-state memories. Magnetic tunnel junctions themselves can form a non-volatile memory cell and proposals for an MTJ based magnetic random access memory (MRAM) date from the mid 1990s. The first MTJ based MRAM was demonstrated by IBM in 1999. Today there is much excitement about the potential of MRAM for high density applications and for replacing conventional charge based memories such as DRAM, e-DRAM and even SRAM. These latter technologies may have difficulties scaling to dimensions below 10–15 nm. However, just like sensors, the success of MRAM is predicated on the discovery of new materials with the needed combination of properties for this application. For MRAM, in addition to high tunneling magnetoresistance, it must be possible to switch the magnetic state of the MTJ memory element using tiny currents passed through the MTJ that take advantage of the phenomenon of spin-momentum transfer. This requires MTJ elements in which the magnetic moment of each of the magnetic electrodes in the device are oriented perpendicular to the layers forming the tunneling junction. Moreover, these MTJ elements must be sufficiently stable against thermal fluctuations that their memory, namely the direction of magnetization of the electrode in

which the data is stored, can be sustained for a decade or longer. It is challenging to find materials that can meet these stringent requirements.

This book focuses on classes of materials that exhibit half-metallicity and which have the potential for advanced sensor and memory applications. Half-metallicity is found in magnetic materials in which one of the spin-polarized bands has a band-gap at the Fermi energy and in which the other exchange-split band has a non-zero density of states at the Fermi energy. Examples include members of the perovskite and double-perovskite families, as well as  $\text{CrO}_2$ , and members of the Heusler family of compounds. The oxides typically have magnetic ordering temperatures near or below room temperature but the Heusler compounds can have Curie temperatures that exceed 1,000 K. For example,  $\text{Co}_2\text{FeSi}$  was discovered to have a Curie temperature greater than 1,120 K in 2005. Over the past decade “*simple rules*” for understanding the properties of the vast class of Heusler and half-Heusler compounds have been developed, allowing for systematic materials engineering of such materials for a variety of applications including magnetic sensors and memories. Out of the scope of this book are applications of Heuslers to, for example, thermoelectrics and solar cells. The application of Heuslers to the field of spintronics perhaps began with the inverse design of the quaternary compound,  $\text{Co}_2\text{Cr}_{0.6}\text{Fe}_{0.4}\text{Al}$ , by the Mainz group in 2000. Using the “*simple rules*” mentioned previously to identify potentially Heusler compounds that would not only exhibit high tunneling spin polarization by virtue of their half-metallic character, but at temperatures needed for sensor and memory applications, the Mainz group carried out density functional theoretical modeling of the electronic structure of hundreds of Heusler compounds. They calculated and then experimentally demonstrated that in  $\text{Co}_2\text{Cr}_{0.6}\text{Fe}_{0.4}\text{Al}$  the Fermi energy would lie in the middle of the electronic band-gap in the minority spin-polarized channel. Thus, the half-metallic nature of this material is less sensitive to thermal excitations of minority spin-polarized carriers, so ensuring near complete half-metallicity over the temperature range of applications.

This book provides an insight into our current understanding of Heusler compounds. A detailed understanding of the relationship between their crystal structure and electronic properties is discussed including the influence of atomic disorder. The current state of the art of Heusler based devices is also presented. Of particular importance are Heusler compounds including as one of their constituent elements cobalt for the magnetic electrodes in spin-valve and magnetic tunnel junction devices. These compounds have very high magnetic ordering temperatures, as mentioned above. An important recent focus of interest is the exploration of tetragonally distorted Heusler compounds, and  $\text{Mn}_3\text{Ga}$  and cousins, which display very large values of perpendicular magnetic anisotropy. Such materials have significant potential for spin transfer torque-MRAM.

The detailed understanding of the properties of complex materials such as Heusler compounds and oxides that is described in this book attests to the very bright future of half-metallic materials!

# Preface

Spintronics is the child of magnetoelectronics, which was born with the discovery of the “*half-metallic ferromagnets*” in 1983 by Robert de Groot for NiMnSb and by Jürgen Kübler for Co<sub>2</sub>MnAl and Co<sub>2</sub>MnSn. Peculiar for this type of ferromagnets is that only electrons with one kind of spin take part in the electronic transport properties. This leads to the idea that electronic devices can be built where not the charge but the spin of the electron transports the signal and is thus free of “ohmic” energy dissipation. The exceptional property that the materials exhibit 100 % spin polarization at the Fermi energy makes them ideal candidates for spin injection devices to be used in spin electronics that is spintronics.

Spintronics is an emerging technology exploiting the spin degree of freedom and has proved to be very promising for new types of fast electronic device. Amongst the anticipated advantages of spintronics technologies, researchers have identified the non-volatile storage of data with high density and low energy consumption as particularly relevant. This monograph examines the concept of half-metallic compounds perspectives to obtain novel solutions, and discusses several oxides as well as the intermetallic Heusler compounds. Such materials can be designed and made with high spin polarization and, especially in the case of Heusler compounds, many material-related problems present in current-day 3d metal systems, can be overcome. From materials design by theoretical methods and the preparation and properties of the materials to the production of thin films and devices, this monograph provides an insight into the current research on Heusler compounds and double perovskites. It offers a general understanding of structure–property relationships, including the influence of disorder and correlations on the electronic structure and interfaces. Last not least, spintronics devices such as magnetic tunnel junctions (MTJs) and giant magnetoresistance (GMR) devices, with current perpendicular to the plane, in which Co<sub>2</sub> based Heusler compounds are used as new electrode materials, are also introduced.

The way from materials design to applications and devices is reviewed in 17 chapters by experts in the field. An introduction to Heusler compounds (Chaps. 1–3) and double perovskites (Chap. 4) as materials for spintronics is given in the first four chapters. In the following four chapters, the basic theoretical considerations

for materials design of the half-metallicity of Heusler compounds (Chaps. 5–7) and double perovskites (Chaps. 5 and 8) are given. Next five chapters are devoted to the application of new and well established experiments to investigate the materials and devices (Chaps. 9–13). Finally, four chapters (14–17) review the successful use of the new materials in thin films and devices.

The first part is devoted to new materials from the classes of Heusler compounds and double perovskites. Chapter 1 gives an overview on functionalities and applications of Heusler compounds. The following Chap. 2 reports on new Heusler compounds and their properties starting with material design from the viewpoint of a chemist based on optimization and tuning of the Fermi energy by chemical substitution. Details of crystallographic order and disorder phenomena in Heusler compounds are discussed in Chap. 3. These phenomena are important for an understanding of the structure to property relations. Substitution effects in double perovskites are reported in Chap. 4, which investigates the influence of electron and hole doping in half-metallic  $\text{Sr}_2\text{FeReO}_6$ .

The second part reviews the design of new materials by theoretical methods. Chapter 5 deals with the theory of the half-metallic materials and reviews the half-metallic ferromagnets and ferrimagnets found in the classes of Heusler compounds and double perovskites. The special focus of this chapter is on electronic structure, nature of the magnetic moments and physics of the energy gap for a single spin channel. Chapter 6 is about correlation and chemical disorder in Heusler alloys with a special emphasis on spectroscopic studies. It is shown that effects of local electronic correlations and alloying on the properties of the Heusler compounds need an equal treatment of static and dynamic correlations. More details of the electronic structure of the half-metallic, transition metal based Heusler compounds are reviewed in Chap. 7. It reports on calculation of electronic structure and properties by means of ab-initio band structure methods for ordered, substituted and disordered Heusler compounds. The theory of the electronic structure of complex oxides is reported in Chap. 8, which discusses—based on dynamical mean field theory—the electronic structure, magnetic properties, and metal–insulator transitions in transition metal oxides.

The third part is devoted to new experimental methods and their application to the investigation of new materials. Chapter 9 is about the experimental investigation of the local structure of highly spin polarized Heusler compounds revealed by nuclear magnetic resonance spectroscopy (NMR). It shows that NMR, as a local probe, is a suitable tool to reveal structural contributions and foreign phases in spin polarized materials which are very difficult to detect with other methods. Chapter 10 reports on the investigation of new materials with high spin polarization by X-ray magnetic circular dichroism. It explains in an element specific way the spin and orbital magnetic moments of  $\text{Co}_2\text{YZ}$  (bulk and films) and confirms experimentally the tailoring of the Fermi level in quaternary substituted compounds. As a very young experimental method, hard X-ray photoelectron spectroscopy is applied in Chap. 11 to explore the electronic structure of new materials, thin films, and buried layers in MTJs. In Chap. 12, the surface electronic properties of  $\text{Co}_2\text{Cr}_{1-x}\text{Fe}_x\text{Al}$  are characterized by spin resolved photo emission with low photon energies to discriminate

bulk and surface states. Magneto-optical experiments and ion beam-induced modification of Heusler compounds are reported in Chap. 13 that reports on investigations of magnetic exchange stiffness, magnetic anisotropy, magnetization reversal, and magneto-optical Kerr effect in Co-based Heusler compound thin films.

The last part demonstrates the successful use of new spintronics materials in thin films and devices. Chapter 14 is devoted to a special material ( $\text{Co}_2\text{Fe}(\text{Al}_{1-x}\text{Si}_x)$ ) and its application in spintronics. It reports on the structural and magnetic properties of epitaxial thin films and their applications to magnetic tunnel junctions (MTJs), giant magnetoresistive (GMR) devices and spin transfer magnetization switching. It reveals that the use of Heusler compounds is an effective way to reduce the switching current density in MTJs. Chapter 15 is about the transport properties of  $\text{Co}_2(\text{Mn}, \text{Fe})\text{Si}$  thin films. Especially it is shown that the normal Hall effect undergoes a transition from a hole-like charge transport in  $\text{Co}_2\text{MnSi}$  to an electron-like transport in  $\text{Co}_2\text{FeSi}$ . Chapter 16 reports on the preparation, barrier-interface engineering, and investigation of  $\text{Co}_2\text{Cr}_{1-x}\text{Fe}_x\text{Al}$  thin films for MTJs with  $\text{AlO}_x$  tunneling barriers. The tunnel magnetoresistance in tunnel junctions with  $\text{Co}_2\text{MnSi}$  as Heusler alloy electrode and  $\text{MgO}$  as barrier is investigated in Chap. 17. This completes the way from material design to successful use in spintronics devices.

Mainz, Dresden

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# Acronyms

2-PPE	Two photon photoemission
AAL	Around atomic limit
AF	Antiferromagnetic
AFM	Atomic force microscopy
AP	Antiparallel
APS	Appearance potential spectroscopy
ARUPS	Angular resolved ultraviolet photoelectron spectroscopy
ASA	Atomic sphere approximation
BC-MIT	Bandwidth controlled metal–insulator transition
BIS	Bremsstrahlung isochromat spectroscopy
BL	Beamline
BLS	Brillouin light scattering
CCFA	$\text{Co}_2\text{Cr}_{0,6}\text{Fe}_{0,4}\text{Al}$
CDMFT	Cluster dynamical mean field theory
CEMS	Conversion electron Mößbauer spectroscopy
CMR	Colossal magnetoresistance
COHP	Crystal orbital Hamiltonian population
CPA	Coherent potential approximation
CPP	Current perpendicular to plane
CPP-SV	Current perpendicular to plane spin valves
CPP-GMR	Current perpendicular to plane giant magnetoresistance
DE	Damon–Eshbach
DE	Double exchange
DFT	Density functional theory
DOS	Density of states
DIPS	Digital Image Processing System
DMFT	Dynamical mean field theory
DP	Double perovskite
DSC	Differential scanning calorimetry
EB	Electron beam
EB-MTJ	Magnetic tunneling junction with electron beam evaporated MgO barrier

EDX	Energy dispersive X-ray spectroscopy
EXAFS	Extended X-ray absorption fine structure spectroscopy
FC-MIT	Filling-controlled metal–insulator transition
FID	Free induction decay
FLAPW	Full potential linearized augmented plane-wave
FLEX	Local fluctuating exchange
FM	Ferromagnetic
FWHM	Full width at half maximum
GGA	Generalized gradient approximation
GMR	Giant magnetoresistance
HAADF	High-angle angular dark field
HAXPES	Hard X-ray photoelectron spectroscopy
HDD	Harddisk drive
HF	Hartree–Fock
HMF	Half-metallic ferromagnet
HRTEM	High resolution transmission electron microscope
HTS	High temperature structure
ICP	Inductively coupled plasma
ICSD	Inorganic crystal structure database
IPT	Iterated perturbation theory
JASRI	Japan synchrotron radiation research institute
KKR	Korringa–Kohn–Rostoker
LDA	Local density approximation
LDA+ <i>U</i>	Local density approximation with added correlation potential
LDAD	Linear dichroism in the angular distribution
LDOS	Local density of states
LEED	Low energy electron diffraction
LH	Lower Hubbard
LHB	Lower Hubbard band
LMDAD	Linear magnetic dichroism in the angular distribution
LMOKE	Linear or longitudinal MOKE
LMTO	Linearized muffin-tin orbital
LNLS	Brazilian synchrotron light laboratory
LSDA	Local spin density approximation
LTS	Low temperature
LTS	Low temperature structure
MCDAD	Magnetic circular dichroism in the angular distribution
MDAD	Magnetic dichroism in the angular distribution
MIT	Metal–insulator transition
MOKE	Magneto optical Kerr effect
MR	Magnetoresistance
MRAM	Magnetic random access memory
MTJ	Magnetic tunnel junction
NCA	Non-crossing approximation
NQP	Non-quasiparticle



PDOS	Partial density of states
PMA	Perpendicular magnetic anisotropy
PSV	Pseudo spin valve
QMC	Quantum Monte Carlo
QMOKE	Quadratic magneto-optical Kerr effect
RA	Resistance area
$RA_P$	Resistance area for parallel magnetization configuration
RE	Rare earth
RF	Radio frequency
RHEED	Reflection high energy electron diffraction
RKKY	Rudermann–Kittel–Kasuya–Yosida
RRR	Residual resistivity ratio
RT	Room temperature
SB	Strukturberichte
SE	Superexchange
SEM	Scanning electron microscope
SIC	Self interaction correction
SIC-LDA	Self interaction corrected local density functional approximation
SOC	Spin–orbit coupling
SPEAR	Stanford synchrotron radiation laboratory
SP-MTJ	Magnetic tunneling junction with sputtered MgO barrier
SPRKKR	Spin polarized, full relativistic Korringa–Kohn–Rostocker method
SPTF	Spin polarized T-matrix plus fluctuation
SQUID	Superconducting quantum interference device
SR-PES	Spin resolved photoelectron spectroscopy
TEM	Transmission electron microscopy
TEY	Total electron yield
TM	Transmission
TMO	Transition metal oxides
TMR	Tunneling magnetoresistance
UH	Upper Hubbard
UHB	Upper Hubbard band
UPS	Ultraviolet photoelectron spectroscopy
VSM	Vibrating sample magnetometer
VB-XPS	Valence band photoemission spectra
XAFS	X-ray absorption fine structure spectroscopy
XAS	X-ray absorption spectroscopy
XMCD	X-ray magnetic circular dichroism
XPS	X-ray photoelectron spectroscopy
XRD	X-ray diffraction