

Contents

Preface	ix
Volume Preface	xiii
Chapter 1. GMR in Metallic Multilayers – A Simple Picture	1
1.1. Introduction	1
1.1.1 Nobel prize	1
1.1.2 Magnetoresistance	1
1.1.3 Magnetic recording	3
1.1.4 Perpendicular recording and future storage technology	6
1.2. GMR: A historical perspective	8
1.3. Qualitative arguments	10
1.3.1 Quantum well (QW) approach	11
1.3.2 Spin-polarized quantum well states	11
1.4. Interlayer exchange coupling	15
1.5. 3-dimensional model: Fermi surface nesting	16
1.6. Strength of coupling: theory vs experiment	17
1.6.1 Growth related issues and measuring interlayer coupling	17
1.6.2 GMR in magnetic sensors	19
1.6.3 Biquadratic coupling	20
1.7. Selected multilayer systems	21
1.7.1 Co/Cu(001)	21
1.7.2 Multilayers grown on Fe whiskers	22
1.7.3 Fe/Cr system	23
1.7.4 Multilayered alloys and nanowires	23
1.8. Scattering of electrons: a simple picture	25
1.9. Magnetic tunnel junctions	28
1.10. Half-metallic systems	29
1.11. Summary	29
Acknowledgements	30
References	30
Chapter 2. Overview of First Principles Theory: Metallic Films	33
2.1. First principles band structure	34
2.1.1 Linearization in energy	35

2.1.2	Basis sets for thin metallic films	36
2.1.3	Full potential	39
2.1.4	Some aspects of group theory	39
2.1.5	Simple examples	42
2.1.6	Spectral representation	43
2.2.	Density functional theory: reduction of the many-electron problem	44
2.3.	Itinerant magnetism	45
2.4.	Localized vs. itinerant magnetic moments	46
2.5.	Stoner criteria	47
2.6.	RKKY theory and interlayer coupling	48
2.7.	Local spin-density functionals	52
2.8.	Helical magnetic configurations: non-collinear magnetism	54
2.9.	Orbital and multiplet effects	55
2.10.	Current density functional theory	57
2.10.1	Current density in exchange–correlation of atomic states	58
	References	59
Chapter 3. Thin Epitaxial Films: Insights from Theory and Experiment		63
3.1.	Metastability and pseudomorphic growth	63
3.2.	A brief introduction to kinetics	64
3.3.	Strain in hetero-epitaxial growth	65
3.4.	Alloy phase diagrams and defects	66
3.5.	Metastability and Bain distortions	69
3.6.	Interfaces in metallic multilayers – Pb-Nb and Ag-Nb	73
3.7.	Magnetic 3d metals	76
3.8.	Epitaxially grown magnetic systems	77
3.9.	More on epitaxially grown fcc Fe/Cu	78
3.10.	Epitaxially grown Fe ₁₆ N ₂ films	81
3.10.1	Experimental background: Fe nitrides	82
3.10.2	Discussion of large Fe moments	83
3.11.	More on Fe/Cr	84
3.12.	bcc Nickel grown on Fe and GaAs	85
3.13.	Summary	85
	References	86
Chapter 4. Magnetic Anisotropy in Transition Metal Systems		89
4.1.	Basics of magnetic anisotropy	89
4.1.1	Magnetocrystalline anisotropy (MCA)	90
4.1.2	Early work	91
4.1.3	Dipole–dipole interaction and related anisotropy	92

4.1.4	Magnetoelastic anisotropy	93
4.1.5	Perpendicular magnetic anisotropy	94
4.1.6	XMCD and XMLD for anisotropy measurements	96
4.1.7	Mermin–Wagner theorem	97
4.1.8	Spin Hamiltonian	97
4.1.9	Band theoretical treatments	98
4.1.10	Spin reorientation transitions in multilayers	99
4.2.	Exchange-bias due to exchange anisotropy	101
4.2.1	Exchange anisotropy with insulating AFM films	105
4.2.2	Exchange anisotropy with metallic AFM films	106
4.2.3	Applications: Exchange-biasing in spin-valves/sensors	107
	References	109
Chapter 5. Probing Layered Systems: A Brief Guide to Experimental Techniques		111
5.1.	SMOKE (Surface Magneto-Optic Kerr Effect)	111
5.2.	AES (Auger Electron Spectroscopy)	114
5.3.	FMR (Ferromagnetic Resonance)	115
5.4.	STM (Scanning Tunneling Microscopy)	115
5.5.	AFM (Atomic Force Microscopy)	116
5.6.	Neutron diffraction	117
5.7.	Mössbauer spectroscopy	117
5.8.	LEED (Low Energy Electron Diffraction)	119
5.9.	RHEED (Reflection High Energy Electron Diffraction)	120
5.10.	ARPES (Angle Resolved Photo-Emission Spectroscopy)	122
5.11.	XAS (X-ray absorption spectroscopy)	124
5.12.	Magnetic Dichroism in XAS	125
5.13.	X-PEEM (X-ray Photoelectron Emission Microscopy)	125
5.14.	SPLEEM (Spin Polarized Low Energy Electron Microscopy)	126
5.15.	Andreev reflection	127
	References	129
Chapter 6. Generalized Kohn–Sham Density Functional Theory via Effective Action Formalism		131
6.1.	Introduction	131
6.2.	Effective action functional	133
6.3.	Generalized Kohn–Sham theory via the inversion method	135
6.4.	Kohn–Sham density-functional theory	138
6.4.1	Derivation of Kohn–Sham decomposition	138
6.4.2	Construction of the exchange-correlation functional	140

6.4.3 Kohn–Sham self-consistent procedure	143
6.5. Time-dependent probe	145
6.6. One-electron propagators	147
6.7. Excitation energies	148
6.8. Theorems involving functionals $W[J]$ and $\Gamma[Q]$	151
6.8.1 Time-independent probe	151
6.8.2 Time-dependent probe	153
6.9. Concluding remarks	155
Acknowledgements	155
References	156
Chapter 7. Magnetic Tunnel Junctions and Spin Torques	157
7.1. Magnetic random access memory (MRAM)	157
7.2. Magnetic tunnel junctions	159
7.3. Theoretical aspects of TMR	161
7.4. Devices with large TMR values	163
7.5. Double barriers, vortex domain structures	165
7.6. Spin transfer torques in metallic multilayers	166
7.7. Ultra-fast reversal of magnetization	171
7.8. Transistors based on spin orientation	173
7.9. Summary	173
References	174
Chapter 8. Confined Electronic States in Metallic Multilayers	177
8.1. Wedge shaped samples	178
8.2. Phase accumulation model	179
8.3. Interfacial roughness	182
8.4. Envelope functions of the QW state	182
8.5. Multiple quantum wells	183
8.6. Non-free-electron-like behavior	184
8.7. Reduction of the 3-dimensional Schrödinger equation	185
8.8. Envelope functions and the full problem	187
8.9. Applications – confined states in metallic multilayers	190
8.9.1 Spin transmission and rotations	191
8.9.2 Angle resolved photoemission and inverse photoemission	192
8.10. Summary	193
Acknowledgements	193
References	194

Chapter 9. Half-Metallic Systems: Complete Asymmetry in Spin Transport	195
9.1. Introduction	195
9.1.1 Covalent gaps	198
9.1.2 Charge-transfer gaps	198
9.1.3 d-d band gap materials	198
9.2. Half Heusler alloys: NiMnSb and PtMnSb	198
9.3. Full Heusler alloys: Co_2MnSi , Co_2MnGe , $\text{Co}_2\text{Cr}_{1-x}\text{Fe}_x\text{Al}$	199
9.4. Chromium dioxide	201
9.5. Perovskites and double-perovskites	201
9.6. Multilayers of zincblende half-metals with semiconductors	202
References	202
Chapter 10. Exact Theoretical Studies of Small Hubbard Clusters	205
10.1. Introduction	205
10.2. Methodology and key results	207
10.3. Charge and spin pairings	208
10.4. T-U phase diagram and pressure effects	210
10.5. Unpaired, dormant magnetic state	211
10.6. Linked 4-site clusters	212
10.7. Summary	213
Acknowledgements	214
References	214
Subject Index	217