POLARIZED ELECTRONS IN SURFACE PHYSICS

This page is intentionally left blank

POLARIZED ELECTRONS IN SURFACE PHYSICS

R. Feder



by 106.51.226.7 on 08/04/22. Re-use and distribution is strictly not permitted, except for Open Access articles. Polarized Electrons in Surface Physics Downloaded from www.worldscientific.com

Published by

World Scientific Publishing Co. Pte. Ltd. P. O. Box 128, Farrer Road, Singapore 9128

Library of Congress Cataloging-in-Publication Data is available.

Polarized Electrons in Surface Physics

Copyright © 1985 by World Scientific Publishing Co. Pte. Ltd.

All rights reserved. This book, or parts thereof, may not be reproduced in any form or by any means, electronic or mechanical, including photocopying, recording or any information storage and retrieval system now known or to be invented, without written permission from the Publisher.

ISBN 9971-978-49-0 9971-978-50-4 pbk

CONTENTS

Foreword	xiii
----------	------

Part I: Theoretical Foundation

1.	Elec	tronic a	nd Magnetic Structure of Solid Surfaces	
	A . J	Freem	an, C. L. Fu, S. Ohnishi & M. Weinert	3
	1.1	Introd	luction	5
	1.2	Theor	etical Framework	8
		1.2.1	Local Spin Density Functional Theory	9
		1.2.2	Thin-Slab Approximation	12
	1.3	Appro	bach and Methodology	13
		1.3.1	FLAPW Method for Thin Films	13
		1.3.2	Energetics of Surfaces: All-Electron Total	
			Energy Approach	19
	1.4	Magne	etism of Transition Metal Surfaces	20
		1.4.1	Ferromagnetic Fe(001) Surface	20
		1.4.2	Ferromagnetic Ni(001) Surface	25
		1.4.3	On the Possibility of Surface Magnetism V(001)	29
		1.4.4	Surface Magnetism of Cr(001)	35
		1.4.5	Induced Magnetism and Knight Shift of Pt(001)	41
	1.5	Magne	etism at Bimetallic Interfaces	44
		1.5.1	Magnetism at the Ni/Cu Interface	44
		1.5.2	Magnetism of the Fe(001) Surface Overlayered	
			with Ag	48
	1.6	Effect	s of Adsorbates on Magnetic Surfaces:	
			1)H/Ni(001)	50
	1.7		Dimensional Magnetism of Metallic Overlayers,	
			aces and Superlattices	54
			•	
2.	Ferr	omagne	tism of Transition Metals at Finite Temperatures	
		-	- nn	67
	2.1	•	uction	69
	2.2		Temperature Properties; What Drives the Phase	
			tion?	75

2.3	The Paramagnetic Phase	78
2.4	Concluding Remarks	89

3. Critical Behaviour at Surfaces of Ferromagnets

<i>K. B</i>	inder	93
3.1	Introduction	95
3.2	Mean Field Theory for the Semi-Infinite Ising Model	101
3.3	Scaling Theory and Renormalization Group Results	107
3.4	Monte Carlo Simulations	115
3.5	Summary	121

4. Principles and Theory of Electron Scattering and Photoemission

<i>R</i> . <i>F</i>	'eder		125
4.1	Introd	luction	127
4.2	One-E	Electron Picture	130
	4.2.1	Relativistic Electron-Ferromagnet Hamiltonian	130
	4.2.2	Effective One-Electron Potentials	133
4.3	Elastic	c Low-Energy Electron Scattering	141
	4.3.1	Basic Concepts	141
	4.3.2	Time Reversal and Spatial Symmetries	146
	4.3.3	Single-Site Scattering	151
	4.3.4	General Many-Site Scattering	156
	4.3.5	Diffraction by Two-Dimensionally Periodic Systems	158
	4.3.6	Disorder and Lattice Vibration Effects	164
	4.3.7	Determination of Magnetic and other Surface Properties	165
4.4	Inelast	tic Scattering and Secondary Electron Emission	170
	4.4.1	Loss Mechanisms and Spin-Dependence	171
	4.4.2	Electron-Hole Pair Excitation	173
	4.4.3	Spin Fluctuations	178
	4.4.4	Imaginary Potential and Mean Free Path	181
	4.4.5	True Secondary Electron Emission	183
4.5	Photo	emission	185
	4.5.1	Basic Concepts	186
	4.5.2	General Theoretical Framework	188
	4.5.3	Relativistic One-Step Theory for Ferromagnets	192
	4.5.4	"Golden Rule" Form and Three-Step Model	195
	4.5.5	Nonrelativistic Limit and Electric Dipole Approximation	198

	4.5.6	Non-Magnetic Solids with Spin-Orbit Coupling 201
		4.5.6.1 One-Step-Model Features and Selection Rules 201
		4.5.6.2 Bulk Interband Transitions 214
		4.5.6.3 Transport Effects 218
		4.5.6.4 Surface Transmission
		4.5.6.5 Emission from Adsorbates 224
	4.5.7	Transition Metal Ferromagnets 225
		4.5.7.1 At Low Temperature
		4.5.7.2 Near the Curie Temperature 228
4.6	Brems	sstrahlung (Inverse Photoemission)
	4.6.1	Principles 231
	4.6.2	Theory
4.7	Conclu	uding Remarks

Part II: Experiments and Results

5.	Sources and Detectors for Polarized Electrons							
	J. Kirschner							
	5.1	Source	es of Polarized Electrons 247					
		5.1.1	Introduction					
		5.1.2	Photoemission Sources					
		5.1.3	The Field Emission Source 259					
	5.2	Detect	tors for Polarized Electrons					
		5.2.1	Introduction					
		5.2.2	Mott Detectors					
		5.2.3	The Absorbed Current Detector 271					
		5.2.4	The LEED Detector 276					

6. Elastic Spin-Polarized Low Energy Electron Diffraction from Non-Magnetic Surfaces F. B. Dunning & G. K. Walters 6.1 Introduction 6.2 Spin-Dependent Elastic Scattering – Basic Concepts 6.3 Experimental Considerations

6.4	Experimental Results and Comparisons with Theory				
	6.4.1	Tungsten	01		
		6.4.1.1 $W(001)(1 \times 1) \dots 3$	01		
		6.4.1.2 Adsorbate- and Temperature-Induced			
		Reconstruction	04		
		6.4.1.3 Surface Barrier Resonances	07		

		6.4.2 Gold	309
		6.4.3 Platinum	311
		6.4.4 Nickel	312
		6.4.4.1 Ni(001)	313
		6.4.4.2 Ni(001)c(2×2)Te	314
		6.4.5 Cu ₃ Au: Order-Disorder Transformations	316
	6.5	Conclusions and Future Prospects	318
7.	Elas	tic Spin-Polarized Low-Energy Electron Scattering from	
	Mag	netic Surfaces	
	<i>U</i> . <i>G</i>	Tradmann & S. F. Alvarado	321
	7.1	Introduction: Spin Polarized Electron Scattering in	
		Comparison with other Experimental Probes of Surface	
		Magnetism	323
	7.2	Surface Magnetization of 3d-Magnets at Low Temperatures	326
	7.3	Surface Magnetism and Chemisorption at 3d-Magnet Surfaces	334
	7.4	Critical Behavior of Ni-Surfaces	338
	7.5	Enhanced Surface Curie Temperature and Surface Magnetic	
		Reconstruction of Gd(0001)	341
	7.6	Ferromagnetic Glasses	344
8.		astic Electron Scattering by Ferromagnets	
	J. Ki	irschner	353
	8.1	Introduction	355
	8.2	Spin-Dependence of the Electron Mean Free Path	355
	8.3	Two-Electron Scattering Processes	359
	8.4	Stoner Excitations	365
		8.4.1 Amorphous Glasses	367
		8.4.2 Single Crystals	370
	8.5	Outlook	380
9.	-	Polarized Secondary Electron Emission from Ferromagnets	
	M. L	andolt	385
	9.1	Introduction	387
	9.2	Spin Polarization of True Secondary Electrons	389
		9.2.1 Energy Distribution of the Secondary Electron Spin	
		Polarization	389
		9.2.2 Magnetic Domain Microscopy	394
		9.2.3 Magnetic Depth Profiling	397

9.3	Spin Polarized Auger Spectroscopy	402
	9.3.1 The MMM Auger Process	403
	9.3.2 The LMM Auger Process	409
9.4	Electron Spin Polarization in Inner Shell Excitations in a Solid	412
9.5	Summary	417

10. Spin Polarized Photoemission by Optical Spin Orientation in

Semiconductors

<i>F. M</i>	eier	423
10.1	Introduction	425
10.2	Principles of Optical Spin Orientation in Solids	429
10.3	Applications of Optical Spin Orientation	438
	10.3.1 Hybridization of Energy Bands	438
	10.3.2 Lifting of the Spin-Degeneracy in Non-Centrosymmetric	
	Materials	445
	10.3.3 Structural Phase Transitions	447
	10.3.4 Enhancement of Resolution in Photoelectron Spectro-	
	scopy by Measuring the Spin Polarization	452
	10.3.5 Spin Exchange Scattering	457

11. Spin-Resolved Photoemission from Nonmagnetic Metals and Adsorbates

U. Heinzmann & G. Schönhense 46	7
11.1 Introduction	9
11.2 Energy-, Angle- and Spin-Resolved Photoelectron Emission	
Technique	1
11.2.1 Experimental 47	1
11.2.2 The "Complete" Photoionization Study 47	4
11.3 Symmetry-Resolved Bandmapping of Pt(111) 47	'7
11.3.1 Relativistic Bandstructure	7
11.3.2 Spin-Resolved Photoelectron Spectra and Bandmapping 47	8
11.3.3 Temperature Dependence	0
11.3.4 Comparison with Quantitative Theoretical Calculations 48	52
11.4 Hybridization Effects and Special Regions of Energy Bands 48	5
11.4.1 The W(100) Case	5
11.4.2 The Λ -Direction of Pt and Au	7
11.5 Off-Normal Photoelectron Emission	0
11.5.1 Surface Transmission Effects	0
11.5.2 Dependence of the ESP Vector on the Emission Angle 49	2

	11.6 Photoelectron Spinpolarization Spectroscopy of Physisorbed	
	Rare Gases	495
	11.6.1 Level Splitting	495
	11.6.2 Resonance Behavior of the Spin Polarization	500
	11.6.3 Influence of Substrate, Overlayer Structure and 2D	
	Phase Transitions	504
	11.7 Adsorbate-Induced Changes in Substrate ESP Spectra	506
12.	Spin - and Angle - Resolved Photoemission from Ferromagnets	
	<i>E. Kisker</i>	513
	12.1 Introduction	515
	12.2 Experimental Set-Ups for Spin- and Angle-Resolved	
	Photoemission	518
	12.3 Experimental Results and Discussion	521
	12.3.1 Ni(110)	521
	12.3.2 Fe(100)	524
	12.3.3 Co(110)	528
	12.3.4 Oxygen Adsorption Studies	529
	12.3.5 Auger Electrons and Resonant Photoemission from	
	3d-Transition Metals	530
	12.3.6 Study of the Ferromagnetic to Paramagnetic Phase	
	Transitions of Fe and Ni	534
	12.3.6.1 Introduction	534
	12.3.6.2 Fe(100)	536
	12.3.6.3 Ni(110)	539
	12.4 Concluding Remarks	541
13.	Spin Dependent Inverse Photoemission from Ferromagnets	
	V. Dose & M. Glöbl	547
	13.1 Introduction	549
	13.2 Experimental	551
	13.3 Room Temperature Data for Iron	553
	13.4 Measurements at Elevated Temperature	559
	13.5 Outlook	562
14.	Photoemission and Bremsstrahlung from Fe and Ni:	
	Theoretical Results and Analysis of Experimental Data	
	R. Clauberg & R. Feder	
	14.1 Introduction	567

14.2	Analysis at Low Temperature	567
	14.2.1 Fe(001) and Fe(110)	568
	14.2.2 Ni(110)	577
	14.2.3 Ni(110)(2 × 1)-0	583
14.3	Analysis Near the Curie Temperature	588
]	14.3.1 Fe(001)	589
1	14.3.2 Ni(110)	597
Polariz	zed Electrons in Surface Physics: Outlook	

605

This page is intentionally left blank

Foreword

Surface physics, dealing with physical (and thence also chemical) properties and processes related to the solid/vacuum boundary, has developed into a vast field of still growing scientific and technological importance. (An extensive survey and references may be found in four volumes recently edited by King and Woodruff (1981-1984)). Electrons are essential for surface physics in two respects: firstly, bound electrons are a constituent part of any surface system, essential not only for the very existence of the system (its local bonding and geometry), but also for its vibrational, magnetic and chemical properties; secondly, free electrons provide - in a wide variety of scattering and emission techniques - powerful means of studying surface properties. Particularly interesting and useful phenomena occur, if the ensemble of electrons under consideration is polarized, i.e. if the number of electrons with spin parallel to a preferential direction differs from the number with spin antiparallel. For electrons bound to the surface system, this is associated with ferro- or ferrimagnetic ordering. In electron spectroscopy techniques, one is dealing with a beam of polarized electrons which is incident on the surface or emerges from it. (A general introduction to polarized free electrons and their use in atomic, solid state and high-energy physics is given in a monograph by Kessler (1976 and, updated, 1985)). Interacting with the surface system via exchange or spin-orbit coupling, polarized electron beams have - due to substantial advances in producing them ("sources") and analysing their spin polarization ("detectors") - within the past decade established themselves as a unique tool for studying magnetic, electronic and even geometrical surface properties.

In view of the achievements already made, the rapidly growing interest in and the future promise of this field, the time appears ripe for a comprehensive presentation, which initiates the non-specialist (with a general physics background at the graduate level) and reviews the current state of the art. This is the aim of the present book. It consists of a coherent sequence of fourteen chapters written by top level experts, who have significantly promoted progress in the respective sub-areas of the field.

The book is organized in two main parts: (I) theoretical foundation, (II) experiments and (experimental and theoretical) results.

Part I (Chapters 1 to 4) introduces fundamental concepts and theoretical approaches. Chapter 1 is devoted to the electronic and magnetic structure of clean and adsorbate-covered surfaces at temperatures well below their ferromagnetic transition temperature. After setting the theoretical framework of local spin-density-functional formalism and thin film approximation, the currently most fruitful first-principles theory for calculating the spin-polarized electronic ground state is introduced, and numerical results for a variety of typical transition metal surfaces and overlayers are presented and discussed. While ferromagnetism of the infinite solid ("bulk") at low temperatures is well understood (in particular itinerant Stoner model for 3d transition metals and Heisenberg Model for rare-earth systems) (cf. standard textbooks on Solid State Physics, e.g. Ashcroft and Mermin (1976), Callaway (1976), Harrison (1970)), transition metal ferromagnetism near the Curie temperature is a subject of very recent controversy and progress. Since an understanding of the "bulk" is a prerequisite for understanding the surface, and since polarized electrons (in photoemission) have provided valuable new insight, key concepts (spin fluctuations, local moments, short-range magnetic order) and theoretical state of the art are therefore included in the present book (Chapter 2). This is naturally followed by a survey of surface ferromagnetism near the Curie temperature (Chapter 3), i.e. "critical behaviour", including scaling theory, renormalization group and Monte Carlo simulations. Chapters 1 to 3 having dealt with the spin-polarized (ferromagnetic) structure of surface systems "by themselves", Chapter 4 addresses the interaction of polarized free electrons with magnetic and non-magnetic surface systems

(semi-infinite solid with clean or adsorbate-covered surface), which is fundamental to a wide variety of electron scattering and emission techniques for investigating surface properties. Observable spin polarization effects may arise from ferromagnetic exchange interaction and/ or from spin-orbit coupling, which are both formally incorporated in a one-electron Dirac Hamiltonian containing an effective magnetic field. The theory of elastic spin-polarized low-energy electron diffraction (LEED) is presented in some detail, firstly because of its intrinsic importance and secondly because the "LEED state" (or its time reverse) is an essential ingredient for quantitative theories of other methods like photoemission, inverse photoemission and inelastic electron scattering, which are subsequently discussed. General results due to symmetry properties are presented, and principles of deducing, with the aid of theory, surface properties from experimental data are explained.

Part II (Chapters 5 to 14) deals with experimental techniques, experimental results and physical information obtained by comparing experimental data with their theoretical counterparts. Chapter 5 introduces the essential experimental tools: sources of polarized electrons, spin polarization detectors (polarimeters), synchrotron radiation (linearly and circularly polarized) and photon detectors. Elastic spinpolarized low-energy electron diffraction is presented for non-magnetic and for ferromagnetic surfaces in Chapters 6 and 7, respectively. In particular, the determination of the surface geometry, of the layerdependent-magnetization at low temperatures and of the ferromagnetic critical behaviour of surfaces is illustrated. The subsequent two Chapters are devoted to spin-dependent electron-electron collision processes. The techniques, which are presented, include in particular high-resolution electron energy loss spectroscopy from ferromagnets, culminating in a "triple scattering" experiment involving both a polarized primary beam and spin analysis of inelastically scattered electrons (Chapter 8), and secondary electron emission (especially Auger emission and the very-low-energy "cascade") (Chapter 9). In addition to revealing details of the electron-electron interaction and ferromagnetic surface and bulk properties, these studies have led to the technologically important development of a magnetic scanning electron microscope. Chapters 10 to 12 are devoted to spin-resolved photoemission due to radiation in the (vacuum) ultraviolet range (photon energies up to about 70 eV). Chapter 10 focuses on semiconductor surfaces, for which spin-orbit coupling together with circular light polarization produces highly polarized photoelectrons, which carry information on the bulk band structure, on doping with impurities and - due to a most recently discovered spin precession effect in non-centrosymmetric crystals - on the spatial extent of the band-bending region near the surface. For non-magnetic metal surfaces, spin-, angle- and energy-resolved photoemission experiments performed with circularly polarized ultraviolet synchrotron radiation permit a direct observation of the symmetry types of the occupied states and promise detailed information on the electronic structure of adsorbed overlayers (Chapter 11). For ferromagnets (Chapter 12), spin-resolved photoemission by linearly polarized or unpolarized light reveals the majority- and minority-spin (quasi-particle) bulk and surface band structures. While photoemission observes the occupied electronic states, its inverse, bremsstrahlung induced by polarized electrons (Chapter 13), provides complementary information on the unoccupied states (in particular in the vicinity of the Fermi level). The retrieval of physical information from experimental photoemission and bremsstrahlung data by means of theoretical model calculations is illustrated in Chapter 14 for ferromagnetic Fe and Ni. In particular, the determination of short-range magnetic order near the Curie temperature is demonstrated, and some light is shed on the influence of chemisorption on surface magnetism. The final Chapter 15 gives a synopsis and an outlook on future prospects for polarized electrons both in fundamental surface physics research and in technological applications.

The organization of Part II is such that physical properties of specific materials are presented in conjunction with the polarizedelectron method by which they were revealed. An alternative classification of the results according to materials is indicated in the following "cross reference" table, which may also serve as a Reader's guide to Chapters 6 to 14.

Material	ferromagnetic		non-magnetic		
Method	meta 3d	als 4f	non- metals	metals	semi- conductors
elastic scattering	7	7		6	
inelastic scattering	8	8		8	
secondary emission	9		9	9	
photoemission	12,14	12	12	11	10
bremsstrahlung	13,14				

Table: Chapters, in which results for different types of material as obtained by polarized-electron methods are presented.

Having outlined the scope and contents of the present book, it seems pertinent to briefly mention some related methods for studying ferromagnetic surfaces, which have not been included. About a decade ago, a substantial research effort was devoted to field emission, i.e. to extracting polarized electrons from ferromagnets by applying a strong electric field (for reviews and references cf. Kessler 1976 and 1985, Campagna et al. 1976, Feuchtwang et al. 1978, Celotta and Pierce 1980). The development of spin-, angle- and energy-resolved photoemission (cf. Chapters 10-12) has, however, superseded field emission as a magnetic surface diagnostic technique, and the polarizedelectron source based on field emission from an EuS-coated W tip has - despite its merits of about 90 % polarization and high brightness not survived in the competition against the presently most widely used and even commercially available GaAs-photoemission source (cf. Chapter 5). Polarized field emission has therefore - to our knowledge - not been pursued further since about 1980, and belongs to the history

Since we concentrate on techniques involving free polarized electrons, tunneling between superconductors and ferromagnets (cf. e.g. Tedrow et al 1982, Feuchtwang et al. 1978), which yields information on the spin polarization of electron states very close to the Fermi energy, has not been included. For the same reason, Mössbauer spectroscopy (cf. review by Keune 1985) is not represented nor is another interesting nuclear-physics method known as "Electron Capture Spectroscopy" (cf. review by Rau 1982) , in which deuterons impinging at grazing angles on a ferromagnetic surface pick up conduction electrons and thus carry information on surface magnetism. Another recent technique, which yet has to prove its quantitative merits, employs a polarized beam of low-energy positrons and measures the spin dependence of the positronium formation rate at the magnetic surface (Gidley et al. 1982) (cf. also a monograph on positron studies: ed. Mills and Canter 1985). Further, an atomic-physics method, in which spin-polarized metastable atoms are ionized at a ferromagnetic surface and subsequently neutralized in a polarization-dependent conduction-band Auger process, appears promising (Onnelion et al. 1984).

In conclusion of this Foreword, may we express a personal thought? The authors hope that the book is not only useful and enjoyable to you, dear Reader, but that you may also share some of their enthusiasm about this flourishing area of surface physics.

Roland Feder

of surface physics.

References

- Ashcroft N W and Mermin N D 1976 Solid State Physics (Holt, Rinehart and Winston, New York)
- Callaway J 1976 Quantum Theory of the Solid State (Academic Press, New York)
- Campagna M, Pierce D T, Meier F, Sattler K and Siegmann H C 1976 Adv. El. and El. Physics <u>41</u> 113
- Celotta R J and Pierce D T 1980 in Adv. in Atomic and Molecular Physics 16 101
- Feuchtwang T E, Cutler P H and Schmit J 1978 Surface Sci. 75 401
- Gidley D W, Koymen A R and Capehart T W 1982 Phys. Rev. Lett. 49 1779
- Harrison W A 1970 Solid State Theory (McGraw Hill, New York)
- Kessler J 1976/1985 Polarized Electrons (Springer, Berlin Heidelberg New York)
- Keune W 1985 in Proceedings of the International Conference on Applications of the Mößbauer Effect, Leuven, Sept. 1985, in "Hyperfine Interactions" (North Holland, Amsterdam)
- King D A and Woodruff D P 1981-85 (ed) The Chemical Physics of Solid Surfaces and Heterogeneous Catalysis (North Holland, Amsterdam)
- Mills A and Canter K F (ed) 1985 Positron Studies of Solids, Surfaces and Atoms (World Scientific Publishing Co, Singapore 1985)
- Onellion M, Hart M W, Dunning F B and Walters G K 1984 Phys. Rev. Lett. 52 380
- Rau C 1982 J. Magn. Magn. Mater. 30 141
- Tedrow P M, Moodera J S and Meservey R 1982 Solid State Commun. 44 587