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Atomic Scale Engineering by Forces and Currents

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Preface

This monograph on scanning probe microscopes (SPM) has three aims: to present, in a coherent way, the theoretical methods necessary to interpret experiments; to demonstrate how experimental results are in fact enhanced by theoretical analysis; and to describe the physical processes in solids that can be analyzed by this experimental method. In all these aims we focus on high-resolution experiments as the cutting edge in SPM, offering access to physical phenomena at the atomic scale.

The presentation is directed at an audience of practitioners in the field and newcomers alike. For one group, it presents an overview of methods, which are found in a widely disparate range of publications. Moreover, the immediate relevance for the physics of scanning probe microscopes is not usually obvious. For these practitioners, we aim at providing them with a toolbox that can be used in conjunction with existing numerical methods in solid state physics. For the other group, we seek to define the range of phenomena in solid state physics where scanning probe microscopes provide the best analytical tool at present. We also aim at demonstrating, in a step-by-step fashion, how physical problems in this field can be treated experimentally, and clarified with the help of state-of-the-art theoretical methods.

The monograph has four distinct parts: Part I, which includes Chapters 1 and 2, covers the basic physical principles and the experimental implementation of the instrument. Part II, Chapters 3–5, contains the core of the theoretical framework. Part III, Chapters 6–9, explains how the theoretical results can be used to analyze experimental data. We conclude the presentation with an outlook on the field, as it presents itself today, and try to estimate its potential development in the near future.

A systematic study of the present state in scanning probe microscopy is impossible without help from a large number of experimenters and theorists. In this respect the authors are grateful to their collaborators over the years in the field, and for the insights gained in many discussions. In particular we would like to thank the following individuals:

Wolf Allers, Andres Arnau, Clemens Barth, Alexis Baratoff, Roland Bennewitz, Richard Berndt, Flemming Besenbacher, Matthias Bode, Harald Brune, Giovanni Comelli, Pedro Echenique, Sam Fain, Roman Fasel, Andrew Fisher, Fernando Flores, Andrey Gal, Aran Garcia-Lekue, Franz Giessibl, Sebastian Gritschneder, Peter Grutter, Claude Henry, Regina Hoffmann, Lev Kantorovich, Josef Kirschner, Jeppe Lauritsen, Petri Lehtinen, Alexander Livshits, Christian Loppacher, Nicolas Lorente, Edvin Lundgren, Ernst Meyer, Rodolfo Miranda, Herve Ness, Risto Nieminen, Georg Olesen, Riku Oja, Olli Pakarinen, Krisztian Palotas, Ruben Pérez, John Pethica, John Polanyi, Josef Redinger, Michael Reichling, Jeff Reimers, Neville Richardson, Federico Rosei, Alexander Shluger, Alexander Schwarz, Udo Schwarz, Peter Sushko, Peter Varga, Matt Watkins, Roland Wiesendanger, and Robert Wolkow.
A first draft of the book was sent out to several colleagues for their comments, criticism, and suggestions for possible improvements. Their feedback was invaluable for improving and clarifying the presentation, both from a theoretical angle, and from the viewpoint of experiments. We would like to thank them particularly for the time and effort they devoted to this careful reading.

Contents

Mathematical Symbols

Symbol	Name	Unit	Chapter
V	Bias potential	volt (V)	4
B	Magnetic field	tesla (T) = V s/m^2	3
μ	Magnetic moment	$\mu_B = e\hbar/2mc$	3
	Chemical potential	eV	4
H	Hamiltonian	eV	3
ψ_μ,χ_ν	Eigenvector	(1/Å)$^{3/2}$	3
$\Gamma\mu\nu$	Transition rate	1/s	3
Γ	Contact	eV	4
I, $I_{\mu\nu}$	Current	ampere (A)	3
E_μ, E_ν	Eigenvalues	eV	3
E_F	Fermi energy	eV	4
σ	Broadening	eV	3
$\rho(\mathbf{r})$, $n(\mathbf{r})$	Electron density	(1/Å)^3	3
k	Electron wavevector, mode	1/Å	4
k_F	Fermi wavevector	1/Å	4
$f(E)$	Fermi distribution	unity	4
v_k	Electron velocity	m/s	4
R_C	Contact resistance	ohm(Ω)	4
G, σ	Conductance	Ω^{-1}	4
Σ	Self energy	eV	4
T	Transmission	unity	4
S	Scattering matrix	unity	4
t	Transmission coefficient	unity	4
r	Reflection coefficient	unity	4
$\bar{T}$	Transmission function	unity	4

Symbol	Name	Unit	Chapter
G_{in}, G_{out}	Incoming and outgoing Green's function	$(\mathrm{eV})^{-1}$	4
$G^R(= G_{out})$	Retarded Green's function (GF)	$(\mathrm{eV})^{-1}$	4
$G^A(= G_{in})$	Advanced Green's function (GF)	$(\mathrm{eV})^{-1}$	4
ϵ_i	Eigenvalue	eV	4
U	Potential	eV	4
Σ^R	Retarded self-energy (SE)	eV	4
Σ^A	Advanced self-energy (SE)	eV	4
Γ_R	Retarded contact	eV	4
Γ_A	Advanced contact	eV	4
A	Spectral function	$(\mathrm{eV})^{-1}$	4
$\Sigma^<$	Nonequilibrium SE (less)	eV	4
$\Sigma^>$	Nonequilibrium SE (more)	eV	4
$G^<$	Nonequilibrium GF (less)	$(\mathrm{eV})^{-1}$	4
$G^>$	Nonequilibrium GF (more)	$(\mathrm{eV})^{-1}$	4
D	Phonon correlation function	eV	4
$\mathbf{J}$	Current density	$\mathrm{A/m^2}$	4
f	Force	newton (N)	3
V	Potential	electron volt (eV)	3
E	Energy	$\mathrm{eV} = 1.6\times10^{-19}$ joule	3
C	Capacitance	farad (F)	3
k	Cantilever spring constant	(N/m)	6
ω_0,f_0	Cantilever equilibrium frequency	(s^{-1})	6
A_0, A	Cantilever amplitude	(m)	6
Q	Quality factor	unity	6
U_{bias}	Compensating bias in SFM	(V)	6
H	Hamaker constant	(joule)	6
R	Tip radius	(m)	6
h	Equilibrium height of cantilever	(m)	6
Δf	Frequency shift	(Hz)	6
γ_0	Normalized frequency shift	$(\mathrm{fN}\sqrt{m})$	6