

Synchrotron Radiation

Learn about the properties of synchrotron radiation and its wide range of applications in physics, materials science and chemistry with this invaluable reference. This thorough text describes the physical principles of the subject, its source and methods of delivery to the sample, as well as the different techniques that use synchrotron radiation to analyse the electronic properties and structure of crystalline and non-crystalline materials and surfaces. It explains applications to study the structure and electronic properties of materials on a microscopic, nanoscopic and atomic scale. This book is an excellent resource for current and future users of these facilities, showing how the available techniques can complement information obtained in users' home laboratories, and is perfect for graduate and senior undergraduate students taking specialist courses in synchrotron radiation, in addition to new and established researchers in the field.

D. Phil Woodruff is Emeritus Professor of Physics at Warwick University. He has been awarded a number of prizes for his work in the UK, USA and Germany and is a fellow of the Royal Society. His previous works include *Modern Techniques of Surface Science*, 3rd ed. (Cambridge University Press, 2016).

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Sources and Applications to the Structural
and Electronic Properties of Materials

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Preface

It is now more than 50 years since the first experiments exploiting synchrotron radiation were undertaken on electron synchrotrons designed and operated for experiments in particle physics. These early experiments were mostly conducted by physicists studying photoabsorption, but since that time the range and number of synchrotron radiation facilities, of experimental techniques exploiting this radiation, and of different types of users in chemistry, materials science, engineering, biology and medicine have expanded enormously. Increasingly advanced accelerator physics designs of facilities specifically designed to provide synchrotron radiation, each typically able to accommodate at least 20 different experiments simultaneously, operate as national and international facilities, satisfying the needs of users drawn from this wide range of disciplines. Some of these facility users have, as a particular focus of their research, the development and application of synchrotron radiation techniques, but for the great majority the facility is a (very large) ‘black box’, delivering to them a capability to measure certain properties of their samples that complement other techniques based in their home laboratories.

My own involvement with synchrotron radiation started in the late 1970s through parasitic use of the NINA electron synchrotron at Daresbury in the UK, followed by use of the dedicated synchrotron radiation facilities in Madison, Wisconsin (Tantalus) and near Paris in France (ACO) before returning to Daresbury when the SRS was commissioned. Subsequently, I became a major user of the facilities in Berlin (BESSY and BESSY II) and the ESRF in Grenoble, also running experiments at Brookhaven (NSLS) and Berkeley (ALS) in the USA. During this period I also followed the developments in Trieste (Electra) in Italy and in Lund (from MAX 1 to MAXIV) in Sweden through committee work. My current activities are anchored at the UK’s Diamond facility. This involvement with different facilities, including some aspects of beamline design, and even whole source design (most notably for a facility that was never funded!) convinced me that, for my purposes at least, some understanding of the constraints and capabilities of the storage ring, the insertion devices, and the beamline optics and detectors has helped me to optimise my use of these facilities. I am inclined to believe that many users could benefit from seeing a synchrotron radiation source as rather more than a black box. This was one issue that motivated me to prepare this monograph.

Throughout the book I have tried to focus on the physical principles that underlie all aspects of synchrotron radiation, the actual radiation sources (Chapters 1 and 2);

the beamline optics and other components (Chapter 3); structure determination methods including those that explicitly exploit crystalline periodicity (Chapter 4) and those that do not (Chapter 5); probes of electronic and vibrational structure (Chapters 6 and 7); and finally the broad topic of imaging and micro- and nano-scale analysis that touches on all of these techniques (Chapter 8). I have consciously not covered applications in biological and medical sciences in any depth. These fall too far outside my field of competence for me to understand the significance of the clearly very important applications in these field, although I have included a very small number of examples of applications of general techniques that fall into these areas.

Inevitably, in trying to cover such a wide range of techniques I have benefitted from discussions and correspondence from a number of individuals with expertise complementary to my own. I would particularly like to thank Mike Poole, latterly under difficult circumstances, for much information and advice on accelerator physics and its practical implications, both before and during the writing of this book. I would also like to thank (roughly in the order of the topics as presented in the book) Richard Walker, Elaine Seddon, Ian Robinson, Andy Dent, Christian Morawe, Kevin Cowtan, Laura Gunn, Chiu Tang, Katrin Amann-Winkel, Anders Nilsson, Nick Terrill, Andy Smith, Nathan Cowieson, Phil King, Gerrit van der Laan, Malcolm Cooper, Jon Duffy, George King, Peter Gardner, Brian Tanner and Ian Robinson again, who have kindly provided me with figures from their work and/or improved my understanding of various techniques through further discussions. I hope I have represented their advice fairly. If I failed, the fault is mine, not theirs.

Abbreviations and Acronyms

AFM	atomic force microscopy
APPLE	Advanced Planar Polarised Light Emitter
ARPES	angle-resolved photoelectron spectroscopy
ATR	attenuated total reflection
BESSY	Berliner Elektronenspeicherring-Gesellschaft für Synchrotronstrahlung (Berlin electron storage ring for synchrotron radiation)
BXCDI	Bragg coherent X-ray diffraction imaging
CCD	charge-coupled device
CD	circular dichroism
CHESS	Cornell High Energy Synchrotron Source
Cryo-SXT	cryo-soft X-ray tomography
CT	computed tomography
CXDI	coherent X-ray diffraction imaging
DBA	double bend achromat
DESY	Deutsches Elektronen-Synchrotron (German electron synchrotron facility in Hamburg)
DFT	density functional theory
DOS	density of states
EDAX	energy-dispersive analysis of X-rays
EM	electromagnetic
EPU	elliptically polarising undulator
ERL	energy recovery linac
ESCA	electron spectroscopy for chemical analysis
ESRF	European Synchrotron Radiation Facility (Grenoble, France)
EXAFS	extended X-ray absorption fine structure
FEL	free electron laser
FELIX	Free Electron Laser for Infrared eXperiments
FPA	focal plane array
FTIR	Fourier-transform infrared
GIM	grazing incidence monochromator
HAXPES	hard X-ray photoelectron spectroscopy
HREELS	high resolution electron energy loss spectroscopy
INS	inelastic neutron scattering
LCLS	Linear Coherent Light Source (Stanford, USA)

LEED	low energy electron diffraction
Linac	linear accelerator
MAC	multiple analysing crystal (detector)
MAD	multiple-energy anomalous diffraction
MBA	multi-bend achromat
MIR	multiple isomorphous replacements
MX	macromolecular X-ray crystallography/diffraction
NEXAFS	near-edge X-ray absorption fine structure
NIM	normal incidence monochromator
NIXSW	normal incidence X-ray standing waves
OPD	optical path difference
PCXDI	plane-wave coherent X-ray diffraction imaging
PDF	pair distribution function
PDOS	partial density of states
PEEM	photoelectron emission microscopy
PEPICO	photoelectron–photoion coincidence
PES	photoelectron spectroscopy
PGM	plane grating monochromator
PhD	photoelectron diffraction (energy scan mode)
PSD	position-sensitive detector
PSL	photon-stimulated luminescence
PX	protein X-ray crystallography/diffraction
QEXAFS	quick EXAFS
RAIRS	reflection-absorption infrared spectroscopy
RF	radiofrequency
RIXS	resonant inelastic X-ray scattering
RXES	resonant X-ray emission spectroscopy
SASE	self-amplified spontaneous emission
SAXS	small angle X-ray scattering
SEXAFS	surface EXAFS
SGM	spherical grating monochromator
SLAC	originally Stanford Linear Accelerator Center but now known as SLAC National Accelerator Laboratory
SLS	Swiss Light Source
SNOM	scanning near-field optical microscopy
SPEM	scanning photoelectron microscopy
SRS	Synchrotron Radiation Source (Daresbury, UK)
SSRL	Stanford Synchrotron Radiation Laboratory
STM	scanning tunneling microscopy
SXR	soft X-ray
SXRD	surface X-ray diffraction
TEM	transmission electron microscopy
TGM	toroidal grating monochromator

TOF	time-of-flight
TPES	threshold photoelectron spectroscopy
TPESCO	threshold photoelectron spectroscopy coincidence
TTF	TESLA Test Facility (at DESY)
UPS	ultraviolet photoelectron spectroscopy
UV	ultraviolet
VUV	vacuum ultraviolet
WAXS	wide angle X-ray scattering
XANES	X-ray absorption near-edge structure
XFEL	X-ray free electron laser
XFH	X-ray fluorescence holography
XLD	X-ray linear dichroism
XMCD	X-ray magnetic circular dichroism
XPD	X-ray photoelectron diffraction (angle-scan mode)
XPEEM	X-ray photoelectron emission microscopy
XPS	X-ray photoelectron spectroscopy
XRF	X-ray fluorescence
XRT	X-ray topography
XSW	X-ray standing waves

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