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Theoretical Concepts of X-Ray Nanoscale Analysis

Theory and Applications

Springer

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Preface

X-rays have been proven to be a powerful and reliable tool in studying a large diversity of micro- and nanoscale objects. The wavelength of X-rays is a perfect fit to the typical sizes of basic structures used in all modern technologies and science: crystallographic lattice in semiconductor thin films; biological molecules in protein crystallography; nanoscale objects like quantum dots and quantum wires in optoelectronics; and many others. This fact initiated the intensive development of various measurement techniques and instrumentation to satisfy the large variety of requirements coming from scientific and industrial communities. Information on the intrinsic structure of samples is further obtained from the detailed analysis of the scattered and detected X-ray intensities, which demands robust theoretical methods for data interpretation. The experimental data obtained from modern X-ray equipment contains a large amount of information hidden in the fine structure of the measured X-ray spectra. This fine structure became measurable due to the essential progress in the development of X-ray optics, detectors, and X-ray sources. Explanation of some effects observed in conventional laboratory X-ray measurements requires fundamental investigations which are on the leading edge of a modern science. From another perspective, the application of X-ray methods in production processes requires highly automated and robust analytical tools. Thus, the growing complexity of both experiments and structure of the samples constantly stimulates the further development of the theoretical methods for data analysis.

There are multiple X-ray techniques used for sample evaluation, each of which is suitable for different kinds of the structures. For example X-ray Bragg diffraction probes samples possessing a crystallographic structure and characterizes the structure on a broad scale, from micro-crystallites in polycrystalline materials to the properties of coherent epitaxial samples averaged over large areas. For the latter case of epitaxial structures, X-ray diffraction in a high-resolution mode is used. The information obtained from X-ray diffraction patterns reconstructs the sample morphology, helps in structure determination and phase identification, and may comprise such parameters as crystallinity, mosaicity, crystallographic lattice mismatch, lattice strain status, residual stresses, lattice defects, and many others. The specular X-ray reflectivity characterizes surface and subsurface amorphous or crystalline layers in view of their electron density profiles, layer thicknesses, and interface roughness. The X-ray small-angle scattering

method exposes valuable information on the distribution and characteristics of the non-uniformities inside or on the surface of the sample. In grazing-incidence mode, this technique explores the lateral surface structure of the studied specimens. The pair-distribution function method permits us to obtain the interatomic distances for amorphous, crystalline, and quasi-crystalline materials. The important trend in recent decades is the simultaneous usage of several techniques for characterization, which deliver comprehensive and concise information on the sample structure. However, this approach requires consistent theoretical models of data interpretation for each technique used. This monograph covers the main X-ray techniques used in the material researches, including high-resolution X-ray diffraction, specular and off-specular X-ray reflectivity, grazing-incidence small-angle X-ray scattering, and residual stress analysis. This book presents the unified microscopic approach for a theoretical description of experimental data obtained by various techniques and thus can be used both as a guidance for the development of new interpretation methods in X-ray analysis and as a handbook for students studying the theory of condensed matter and interaction of radiation with the solid state matter.

In addition to the practical aspect of data analysis, the interaction of X-rays with matter plays an important and fundamental role by demonstrating the effectiveness of quantum electrodynamics and scattering theory for the investigation of macroscopic systems. The Hamiltonian describing the interaction of X-rays with atoms has a simple form and contains a small physical parameter proportional to the ratio of the amplitude of Compton scattering of photon on the free electron to the average interatomic distance. As a result, the macroscopic Maxwell's equation for transmission of X-rays in a medium can be derived from first principles after averaging the exact equations of quantum electrodynamics over the microstates of electrons, and without the use of phenomenological material equations. The deduced effective potential of the interaction of X-rays with matter is small enough to successfully use the mathematical methods of the perturbation theory for the scattering problem. This fundamental property of the X-ray optics is not sufficiently covered in the existing literature, and the aim of this book is to illuminate all the theoretical details of the interaction of X-rays with nanoscale objects. The manifestation of the mentioned property of X-ray optics is observed in high-resolution experiments, which are intensively used for the study of thin films and nano-objects possessing a complex structure.

The monograph consists of seven chapters dedicated to different application techniques and fundamental aspects of X-ray scattering from atomic systems. In the Chap. 1, the equations of X-ray optics describing the propagation of a classic wave field in a medium are derived from the Schrödinger equation for the system, which takes into account the quantum properties of both atomistic medium and electromagnetic field. Numerous approximations are discussed, which are used in analytical methods for X-ray optics including calculation of X-ray polarizability. The important aspects of the theory of X-ray scattering from macroscopic objects are considered in the Chap. 2. The relations between the temporal scattering theory of real experiments and the stationary scattering theory with boundary conditions

used in the data interpretation are established. The method of the distorted-wave Born approximation (DWBA) widely used in scattering theory is presented for different sample structures and experimental geometries. The Chap. 3 deals with the method of X-ray reflectivity (XRR) from the multilayered samples with rough interfaces. The theoretical profiles of the specularly reflected X-ray intensity are calculated on the basis of a self-consistent approach for the transition layers at the boundaries of lamellae. The original method of eigenwaves is derived, which simplifies and accelerates the calculation of XRR intensities from the periodic multilayered structures. The basic principles of the high-resolution X-ray diffraction (HRXRD) from the perfect crystalline samples are explained in the Chap. 4. The critical issues of HRXRD are discussed in the details: the transition from kinematical to dynamical theory of X-ray diffraction, the method of eigenwaves for superlattices, the grazing-incidence diffraction (GID), the diffraction from surface nanostructures, and others. The Chap. 5 is dedicated to X-ray diffuse scattering from imperfect surfaces and interfaces. The statistical approach is used to account for the fluctuations of the macroscopic parameters of the sample on the basis of DWBA method. The analysis of the accuracy delivered by different zero approximations for DWBA is performed for the geometry of XRR and grazing-incidence small-angle X-ray scattering (GISAXS) techniques, which are both intensively used for morphology characterization of modern surface nanostructures. X-ray diffraction from the crystals with defects is presented in the Chap. 6, where the attention is paid to the formation and relation between coherent diffraction intensity and diffuse scattering intensity, which is caused by scattering from the statistical ensemble of crystallographic defects. The statistical theory of X-ray diffraction in imperfect crystals is derived, which is applicable for GID case also. The analytical method for simulation of diffuse X-ray peaks caused by the defects is described. This method is applicable for an arbitrary density of the defects existing in the crystal and is comparable in accuracy to the timeconsuming Monte-Carlo calculations. Finally, the Chap. 7 is devoted to the important application of X-rays for residual stress analysis in solid bulk materials, coatings, and polycrystalline samples. The various models of grain interaction are discussed with regard to their applicability limits, and the covariant method of X-ray intensity averaging over the grain distribution is proposed.

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Contents

Acronyms

AFM	Atomic force microscopy
ASF	Atomic scattering factor
DDT	Dynamical diffraction theory
DWBA	Distorted-wave Born approximation
DWF	Debye–Waller factor
EAD	Extremely asymmetric diffraction
GA	Genetic algorithm
GID	Grazing-incidence diffraction
GISAXS	Grazing-incidence small-angle X-ray scattering
GIXRD	Grazing-incidence X-ray diffraction
GTR	Grating truncation rod
HRXRD	High-resolution X-ray diffraction
IR	Irreducible representation
iVW	Inverse Vook–Witt model of grain interaction
MDWBA	Modified distorted-wave Born approximation
MEW	Method of eigenwaves
ODF	Orientation distribution function
PDF	Pair-distribution function
QD	Quantum dots
QED	Quantum electrodynamics
QW	Quantum wires
RDS	Resonant diffuse scattering
RSM	Reciprocal space map
SCA	Self-consistent approach
TER	Total external reflection
VW	Vook–Witt model of grain interaction
XEC	X-ray elastic constants
XFEL	X-ray free electron laser
XRR	X-ray reflectivity
XSF	X-ray stress factors