1. Record Nr. UNINA9910254615703321 Autore Morelhão Sérgio Luiz Titolo Computer Simulation Tools for X-ray Analysis: Scattering and Diffraction Methods / / by Sérgio Luiz Morelhão Cham:,: Springer International Publishing:,: Imprint: Springer,, Pubbl/distr/stampa 2016 **ISBN** 3-319-19554-9 Edizione [1st ed. 2016.] Descrizione fisica 1 online resource (XV, 294 p. 105 illus., 104 illus. in color.) Collana Graduate Texts in Physics, , 1868-4513 Disciplina 548.83 Soggetti Crystallography Materials science Chemistry, Physical and theoretical **Physics** Crystallography and Scattering Methods Characterization and Evaluation of Materials Physical Chemistry Numerical and Computational Physics, Simulation Lingua di pubblicazione Inglese **Formato** Materiale a stampa Livello bibliografico Monografia Note generali Bibliographic Level Mode of Issuance: Monograph Nota di contenuto Radiation-electron (free electron) elementary interaction -- Scattering of X-rays by distributions of free electrons -- Atoms and molecules --X-ray absorption -- Low correlated systems: gases and dilute solutions -- Complex systems I: short-range correlations -- Complex systems II: arbitrary long-range correlations -- Crystals -- Application of kinematic diffraction -- Introduction to dynamical diffraction. The main goal of this book is to break down the huge barrier of Sommario/riassunto difficulties faced by beginners from many fields (Engineering, Physics, Chemistry, Biology, Medicine, Material Science, etc.) in using X-rays as an analytical tool in their research. Besides fundamental concepts. MatLab routines are provided, showing how to test and implement the concepts. The major difficult in analyzing materials by X-ray techniques is that it strongly depends on simulation software. This book teaches the users on how to construct a library of routines to

simulate scattering and diffraction by almost any kind of samples. It

provides to a young student the knowledge that would take more than 20 years to acquire by working on X-rays and relying on the available textbooks. In this book, fundamental concepts in applied X-ray physics are demonstrated through available computer simulation tools. Using MatLab, more than eighty routines are developed for solving the proposed exercises, most of which can be directly used in experimental data analysis. Therefore, besides X-ray physics, this book offers a practical programming course in modern high-level language, with plenty of graphic and mathematical tools.