

Preface

This book is dedicated to students who need to assimilate extensive knowledge in a short period of time. The international scientific production has increased at a breakneck pace, demanding more dynamic approaches and synergies between different areas of knowledge. Mastering X-ray scattering and diffraction methods means to be competent to work in an infinity of areas, studying the various systems where the organizational understanding of matter at the atomic scale is necessary. Since the discovery of X-radiation, its use as an investigative tool has always been in wide expansion provided by advances in instrumental and computational resource. The current development in the fields of medicine and technology has as one of its supporting pillars the structural analysis offered by X radiation. One of the greatest difficulties faced by beginners in the effective use of this fantastic tool is in analyzing the experimental results. Few are the situations where it is possible to extract structural information directly from the experiments. In most situations, computer programs are necessary for simulating the interaction of radiation with matter. The advent of intense radiation sources and the rapid development of nanotechnology constantly create challenges for solutions beyond those offered by the already settled techniques. Preparing new researchers for this scenario of rapid and drastic changes requires more than teaching physical phenomena theories, it also calls for teaching how to implement them in a simple and efficient way. In this book, the fundamental concepts needed to analyze a wide range of materials (macromolecules, liquids, nanoparticles, polymers, amorphous, polycrystals, small-molecule crystals, and protein crystals) using scattering and diffraction techniques are demonstrated through computer simulation tools. The chapters follow an ascending order going from disordered to ordered matter, covering various types of samples and targeting a unification of theoretical approaches. There are exercises that go with each topic presented, which are proposed and solved. There are more than 80 routines in MatLab developed for solving the exercises. Therefore, besides X-ray physics, this book also offers a practical programming course in modern, high-level language with an infinity of graphic and mathematical resources.

Computer Simulation Tools for X-ray Analysis
Scattering and Diffraction Methods

Morelhão, S.L.

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