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Structural Science of Crystalline Polymers Kohji Tashiro, 2022-05-03 This book focuses on the modern development of techniques for analysis of the hierarchical structure of polymers from both the experimental and theoretical points of view. Starting with molecular and crystal symmetry the author explains fundamental and professional methods such as wide and small angle X ray scattering neutron diffraction electron diffraction FTIR and Raman spectroscopy NMR and synchrotron radiation. In addition the author explains another indispensable method computer simulation which includes energy calculation lattice dynamics molecular dynamics and quantum chemistry. These various methods are described in a systematic way so that the reader can utilize them for the purpose of 3D structure analysis of polymers. Not only such analytical knowledge but also the preparation techniques of samples necessary for these measurements and the methods of analyzing the experimental data collected in this way are given in a concrete manner. Examples are offered to help master the principles of how to clarify the static structures and dynamic structural changes in the phase transitions of various kinds of crystalline polymers that are revealed by these novel methods. The examples are quite useful for readers who want to apply these techniques in finding practical solutions to concrete problems that are encountered in their own research. The principal audience for this book is made up of young professional researchers including those working in industry but it can also be used as an excellent reference for graduate level students. This book is the first volume of a two volume set with Structural Science of Crystalline Polymers A Microscopically Viewed Structure Property Relationship being the second volume by the same author.

Molecular Dynamics Simulation J. M. Haile, 1997-03-14 Provides a lot of reading pleasure and many new insights. *Journal of Molecular Structure*. This is the most entertaining stimulating and useful book which can be thoroughly recommended to anyone with an interest in computer simulation. *Contemporary Physics*. A very useful introduction more interesting to read than the often dry equation based texts. *Journal of the American Chemical Society*. Written especially for the novice. Molecular Dynamics Simulation demonstrates how molecular dynamics simulations work and how to perform them focusing on how to devise a model for specific molecules and then how to simulate their movements using a computer. This book provides a collection of methods that until now have been scattered through the literature of the last 25 years. It reviews elements of sampling theory and discusses how modern notions of chaos and nonlinear dynamics explain the workings of molecular dynamics. Stresses easy to use molecules. Provides sample calculations and figures. Includes four complete FORTRAN codes.

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Lea's Chemistry of Cement and Concrete Peter Hewlett, Martin Liska, 2019-03-06 Lea's Chemistry of Cement and Concrete Fifth Edition examines the suitability and durability of different types of cements and concretes their manufacturing techniques and the role that aggregates and additives play in achieving concrete's full potential of delivering a high quality long lasting competitive and sustainable product. Provides a 60% revision over the fourth edition last published in 2004. Includes updated chapters that represent the

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