

Stuart G. Whittington
Editor

Numerical Methods for Polymeric Systems



Springer

Numerical Methods For Polymeric Systems

L Cohen

Numerical Methods For Polymeric Systems:

Numerical Methods for Polymeric Systems Stuart G. Whittington,2012-12-06 Polymers occur in many different states and their physical properties are strongly correlated with their conformations The theoretical investigation of the conformational properties of polymers is a difficult task and numerical methods play an important role in this field This book contains contributions from a workshop on numerical methods for polymeric systems held at the IMA in May 1996 which brought together chemists physicists mathematicians computer scientists and statisticians with a common interest in numerical methods The two major approaches used in the field are molecular dynamics and Monte Carlo methods and the book includes reviews of both approaches as well as applications to particular polymeric systems The molecular dynamics approach solves the Newtonian equations of motion of the polymer giving direct information about the polymer dynamics as well as about static properties The Monte Carlo approaches discussed in this book all involve sampling along a Markov chain defined on the configuration space of the system An important feature of the book is the treatment of Monte Carlo methods including umbrella sampling and multiple Markov chain methods which are useful for strongly interacting systems such as polymers at low temperatures and in compact phases The book is of interest to workers in polymer statistical mechanics and also to a wider audience interested in numerical methods and their application in polymeric systems

Eco-friendly and Smart Polymer Systems Hamid Mirzadeh,Ali Asghar Katbab,2020-05-29 This proceedings book presents the main findings of the 13th International Seminar on Polymer Science and Technology ISPST 2018 which was held at Amirkabir University of Technology Tehran on November 10 22 2018 This forum was the culmination of more than three decades of academic and industrial activities of Iranian scholars and professionals and the participation of many notable international scientists in covering various important polymer related subjects of concern to Iran and the world at large including polymer synthesis processing and properties as well as issues concerning polymer degradation stability and environmental aspects For the past half a century the growing concern for advancing human health quality of life and especially in the last few decades avoiding and combating environmental pollution have shaped and driven scientific activities geared toward the creation of smart materials that are compatible with the human body and have prompted scientists and technologists to pursue research using natural and sustainable sources This book highlights efforts to responsibly address the problems caused by and which can potentially be solved by polymers and plastics

Multiphase Polymer Systems Andreea Irina Barzic,Silvia Ioan,2016-09-19 Phase morphology in multicomponent polymer based systems represents the main physical characteristic that allows for control of the material design and implicitly the development of new plastics Emphasizing properties of these promising new materials in both solution and solid phase this book describes the preparation processing properties and practical implications of advanced multiphase systems from macro to nanoscales It covers a wide range of systems including copolymers polymer blends polymer composites gels interpenetrating polymers and layered polymer metal structures

describing aspects of polymer science engineering and technology The book analyzes experimental and theoretical aspects regarding the thermal and electrical transport phenomena and magnetic properties of crucial importance in advanced technologies It reviews the most recent advances concerning morphological rheological interfacial physical fire resistant thermophysical and biomedical properties of multiphase polymer systems Concomitantly the book deals with basic investigation techniques that are sensitive in elucidating the features of each phase It also discusses the latest research trends that offer new solutions for advanced bio and nanotechnologies Introduces an overview of recent studies in the area of multiphase polymer systems their micro and nanostructural evolutions in advanced technologies and provides future outlooks new challenges and opportunities Discusses multicomponent structures that offer enhanced physical mechanical thermal electrical magnetic and optical properties adapted to current requirements of modern technologies Covers a wide range of materials such as composites blends alloys gels and interpenetrating polymer networks Presents new strategies for controlling the micro and nanomorphology and the mechanical properties of multiphase polymeric materials Describes different applications of multiphase polymeric materials in various fields including automotive aeronautics and space industry displays and medicine

[Variational Methods in Molecular Modeling](#) Jianzhong Wu,2016-12-17 This book presents tutorial overviews for many applications of variational methods to molecular modeling Topics discussed include the Gibbs Bogoliubov Feynman variational principle square gradient models classical density functional theories self consistent field theories phase field methods Ginzburg Landau and Helfrich type phenomenological models dynamical density functional theory and variational Monte Carlo methods Illustrative examples are given to facilitate understanding of the basic concepts and quantitative prediction of the properties and rich behavior of diverse many body systems ranging from inhomogeneous fluids electrolytes and ionic liquids in micropores colloidal dispersions liquid crystals polymer blends lipid membranes microemulsions magnetic materials and high temperature superconductors All chapters are written by leading experts in the field and illustrated with tutorial examples for their practical applications to specific subjects With emphasis placed on physical understanding rather than on rigorous mathematical derivations the content is accessible to graduate students and researchers in the broad areas of materials science and engineering chemistry chemical and biomolecular engineering applied mathematics condensed matter physics without specific training in theoretical physics or calculus of variations

[Polymer Science: A Comprehensive Reference](#) ,2012-12-05 The progress in polymer science is revealed in the chapters of Polymer Science A Comprehensive Reference Ten Volume Set In Volume 1 this is reflected in the improved understanding of the properties of polymers in solution in bulk and in confined situations such as in thin films Volume 2 addresses new characterization techniques such as high resolution optical microscopy scanning probe microscopy and other procedures for surface and interface characterization Volume 3 presents the great progress achieved in precise synthetic polymerization techniques for vinyl monomers to control macromolecular architecture the development of metallocene and

post metallocene catalysis for olefin polymerization new ionic polymerization procedures and atom transfer radical polymerization nitroxide mediated polymerization and reversible addition fragmentation chain transfer systems as the most often used controlled living radical polymerization methods Volume 4 is devoted to kinetics mechanisms and applications of ring opening polymerization of heterocyclic monomers and cycloolefins ROMP as well as to various less common polymerization techniques Polycondensation and non chain polymerizations including dendrimer synthesis and various click procedures are covered in Volume 5 Volume 6 focuses on several aspects of controlled macromolecular architectures and soft nano objects including hybrids and bioconjugates Many of the achievements would have not been possible without new characterization techniques like AFM that allowed direct imaging of single molecules and nano objects with a precision available only recently An entirely new aspect in polymer science is based on the combination of bottom up methods such as polymer synthesis and molecularly programmed self assembly with top down structuring such as lithography and surface templating as presented in Volume 7 It encompasses polymer and nanoparticle assembly in bulk and under confined conditions or influenced by an external field including thin films inorganic organic hybrids or nanofibers Volume 8 expands these concepts focusing on applications in advanced technologies e g in electronic industry and centers on combination with top down approach and functional properties like conductivity Another type of functionality that is of rapidly increasing importance in polymer science is introduced in volume 9 It deals with various aspects of polymers in biology and medicine including the response of living cells and tissue to the contact with biofunctional particles and surfaces The last volume is devoted to the scope and potential provided by environmentally benign and green polymers as well as energy related polymers They discuss new technologies needed for a sustainable economy in our world of limited resources Provides broad and in depth coverage of all aspects of polymer science from synthesis polymerization properties and characterization methods and techniques to nanostructures sustainability and energy and biomedical uses of polymers Provides a definitive source for those entering or researching in this area by integrating the multidisciplinary aspects of the science into one unique up to date reference work Electronic version has complete cross referencing and multi media components Volume editors are world experts in their field including a Nobel Prize winner

Numerical Methods in Laminar and Turbulent Flow ,1987 **Polymer Composites, Nanocomposites** Sabu Thomas,Kuruvilla Joseph,S. K. Malhotra,Koichi Goda,M. S.

Sreekala,2013-04-16 Polymer composites are materials in which the matrix polymer is reinforced with organic inorganic fillers of a definite size and shape leading to enhanced performance of the resultant composite These materials find a wide number of applications in such diverse fields as geotextiles building electronics medical packaging and automobiles This first systematic reference on the topic emphasizes the characteristics and dimension of this reinforcement The authors are leading researchers in the field from academia government industry as well as private research institutions across the globe and adopt a practical approach here covering such aspects as the preparation characterization properties and theory of polymer

composites The book begins by discussing the state of the art new challenges and opportunities of various polymer composite systems Interfacial characterization of the composites is discussed in detail as is the macro and micromechanics of the composites Structure property relationships in various composite systems are explained with the help of theoretical models while processing techniques for various macro to nanocomposite systems and the influence of processing parameters on the properties of the composite are reviewed in detail The characterization of microstructure elastic viscoelastic static and dynamic mechanical thermal tribological rheological optical electrical and barrier properties are highlighted as well as their myriad applications Divided into three volumes Vol 1 Macro and Microcomposites Vol 2 Nanocomposites and Vol 3

Biocomposites *Computational Studies, Nanotechnology, and Solution Thermodynamics of Polymer Systems* Mark D. Dadmun, W. Alexander Van Hook, Donald W. Noid, Yuri B. Melnichenko, Robert G. Sumpter, 2007-05-08 This text is the published version of many of the talks presented at two symposiums held as part of the Southeast Regional Meeting of the American Chemical Society SERMACS in Knoxville TN in October 1999 The symposiums entitled Solution Thermodynamics of Polymers and Computational Polymer Science and Nanotechnology provided outlets to present and discuss problems of current interest to polymer scientists It was thus decided to publish both proceedings in a single volume The first part of this collection contains printed versions of six of the ten talks presented at the Symposium on Solution Thermodynamics of Polymers organized by Yuri B Melnichenko and W Alexander Van Hook The two sessions further described below stimulated interesting and provocative discussions Although not every author chose to contribute to the proceedings volume the papers that are included faithfully represent the scope and quality of the symposium The remaining two sections are based on the symposium on Computational Polymer Science and Nanotechnology organized by Mark D Dadmun, Bobby G Sumpter and Don W Noid A diverse and distinguished group of polymer and materials scientists biochemists chemists and physicists met to discuss recent research in the broad field of computational polymer science and nanotechnology The two day oral session was also complemented by a number of poster presentations The first article of this section is on the important subject of polymer blends M D

Mathematical Reviews, 2006 **Polymer Characterization Techniques and Their Application to Blends** George P. Simon, 2003 This book aims to introduce the reader to a wide range of polymer characterization techniques including thermal rheology mechanical relaxational scattering and spectroscopic analysis In addition to discussing the techniques and their experimental considerations in general the chapters will show how the techniques are applied to polymer systems and how the data obtained is analyzed and interpreted In order to connect each technique to applications each chapter explains the use of the technique in the popular application of polymer blends The blending of polymers continues to be a major area of polymer research in academia and industry and in addition to its instructive role each chapter serves as a review of the blend literature as relevant to a polymer blends researcher **Monte Carlo Simulations for the Structure-property Relationship of Polymers with Complicated Topology** Zhong

Chen,2004 Journal of the Physical Society of Japan ,2009 9th Australasian Fluid Mechanics Conference ,1986
Journal of Experimental and Theoretical Physics ,2004 Encyclopedia of Polymer Science and Engineering ,1985
Dendrite Initiation and Growth in Lithium/polymer Systems Charles William Monroe,2004 Modern Solution Methods for Nonlinear Multidimensional Problems O.M. Belotserkovskii,2000 Preparing the English translation the author has completely revised the Russian edition of 1994 The new versions and generalizations of computational algorithms which were intensively developed by the method of splitting with respect to physical processes are described **Plastic Packaging Materials for Food** Otto G. Piringer,A. L. Baner,2000 Plastic Packaging Materials for Food Barrier Function Mass Transport Quality Assurance and Legislation edited by O G Piringer and A L Baner Plastics have developed into the most important class of packaging materials Their relative impermeability for substances from the surroundings has great influence on the shelf life and the quality of the packed goods At the same time the interaction between the contents and the various components of the packaging plays a decisive role This particular book is indispensable in the search for the optimal plastic packaging It facilitates the estimation of the influence on the goods which come from the surroundings and from the packaging The authors do not restrict themselves only to the description of the phenomena of diffusion or transport in theory but they show what they mean for practical applications Food represents the central theme as main area of application for plastic packaging It can be considered to be the model substance and the findings are to be applied to many other products and systems The main rules and regulations for food packaging of the European Community and the United States are presented in this book Furthermore the authors emphasize the testing methods for proving the mass transport and the sensory check of the quality of the products **Engineered Materials Abstracts** ,1995-04 **Microstructure and Microtribology of Polymer Surfaces** Vladimir Vasil'evich TUSUukruk,2000 Presents 30 of the 62 papers delivered at an August 1998 international symposium in Boston on the tribology of polymeric materials at both the macroscopic and microscopic scales They look at some problems that have arisen as the equipment and experimental techniques for microscopic analysis have outdistanced the ability of scientists to model and interpret the results The overall themes are contact mechanics of polymeric materials micromechanics and microtribology surface microstructures of various polymers and industrial applications Among the specific topics are the role of interfacial slippage in adhesive release the experimental study of the friction regimes on viscoelastic materials sparse coatings by the disperse adsorption of cylindrical brushes and the effect of surface texture on the friction of automotive interior plastics Annotation copyrighted by Book News Inc Portland OR

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