



# Molecular Modeling Of Polymers

**Peter T. Cummings, Phillip Ray  
Westmoreland, Brice Carnahan**



## **Molecular Modeling Of Polymers:**

**Molecular Modeling of Polymers** Gregory C. Rutledge, Doros N. Theodorou, 1998

**Molecular Modeling of Polymer Structures and Properties** Bruce R. Gelin, 1994-01-01 This book provides an introduction to the techniques of molecular modeling and simulation with practical examples

[Molecular Simulation Methods for Predicting Polymer Properties](#) Vassilios Galiatsatos, 2005-02-03 Among the thousands of synthesized polymers new polymeric substances and materials with new often unusual properties often arise Consequently this presents a problem in determining the physical properties of polymers and thus makes it difficult to ascertain how to synthesize polymers with desired properties This book discusses what molecular modelling can do to predict the properties of realistic polymer systems Organized by property each chapter will address the methods one may use to study the particular system Focuses on polymer properties rather than methods making it more accessible to the average scientist engineer All important polymers will be covered such as amorphous polymers semicrystalline polymers elastomers emulsions polymer interfaces and surfaces Chapters contributed by experts in the field Discusses current commercial software used in molecular simulation

**Molecular Modeling of Polymer Free Volume** Derrick B. Callander, 2005 Free volume and free volume distribution have long been used to explain differences in the gas transport properties of polymeric materials However only a few experimental techniques allow a comprehensive evaluation of polymeric void space Through the use of computer simulations the free volume was characterized of two polyester systems used for beverage packaging and polynorbornene a unique polymer with possible applications in both microelectronic fabrication and membrane separations Delaunay Tessellation was used to calculate the fractional free volume FFV of both polyethylene terephthalate PET and polyethylene naphthalate PEN molecular models It was hypothesized that differences in the FFV distributions could be used to explain the higher experimental O<sub>2</sub> solubility in PEN relative to PET The analysis showed that there was no statistical difference between the FFV distributions for O<sub>2</sub> sized penetrants Clustering analysis was performed based upon the tetrahedra formed by Delaunay Tessellation to examine the connectivity of free volume pockets These results show that there is a statistically larger number of small containing less than 10 tetrahedra cluster and between 20 30 3 in volume clusters in PEN It is this difference in small clusters which provides for the 30% higher O<sub>2</sub> solubility in PEN The free volume of a representative high molecular weight amorphous model of Hexafluoroalcohol Substituted Polynorbornene HFA PNB was also characterized in to examine the shape of the free volume cavities and to draw correlations with the mean lifetime of ortho positronium o Ps from Positron Annihilation Lifetime Spectroscopy PALS Delaunay Tessellation and clustering analysis indicated that the free volume clusters in high molecular weight HFA PNB are slightly non spherical Correcting lifetimes for the somewhat non spherical shape of these free volume clusters was insufficient to reproduce experimentally measured positron annihilation lifetimes because the clusters contained many tortuous connections within the clusters Inclusion of this connectivity information does produce a more accurate

estimate of the measured life times This indicates that the o Ps does sample many tetrahedra in these static clusters but does not freely sample every section of these clusters

**Modeling and Simulation in Polymers** Purushottam D. Gujrati, Arkady I. Leonov, 2010-03-30 Filling a gap in the literature and all set to become the standard in this field this monograph begins with a look at computational viscoelastic fluid mechanics and studies of turbulent flows of dilute polymer solutions It then goes on discuss simulations of nanocomposites polymerization kinetics computational approaches for polymers and modeling polyelectrolytes Further sections deal with tire optimization irreversible phenomena in polymers the hydrodynamics of artificial and bacterial flagella as well as modeling and simulation in liquid crystals The result is invaluable reading for polymer and theoretical chemists chemists in industry materials scientists and plastics technologists *Polymer Materials*

Jean Louis Halary, Francoise Laupretre, Lucien Monnerie, 2011-04-04 Advanced reviews for Polymer Materials Molecular modeling of polymers is a subject that cannot be found in any other book in any appreciable detail The detailed chapters on specific polymer systems is a great idea Gregory Odegard Michigan Technological University The polymer community needs a text book which can connect the macroscopic mechanics with mesoscopic and molecular aspects of polymer Liangbin Li University of Science and Technology of China This book takes a unique multi scale approach to the mechanical properties of polymers covering both the macroscopic and molecular levels unlike any other book on the market Based on the authors extensive research and writing in the field Polymer Materials emphasizes the relationships between the chemical structure and the mechanical behavior of polymer materials providing authoritative guidelines for assessing polymer performance under different conditions and the design of new materials Key features of this book include Experimental results on selected examples precede and reinforce the development of theoretical features In depth discussions of a limited number of polymer systems instead of a brief overview of many Self contained chapters with a summary of their key points Comprehensive problems and a solutions manual for the different parts of the book Coverage of the basics with an emphasis on polymer dynamics An indispensable resource for polymer scientists and students alike Polymer Materials is also highly useful for material scientists engineers chemists and physicists in industry and academia Molecular Modeling of High-performance Polymers, 2022 Abstract High performance polymers are extensively used in the aerospace and aeronautics industries due to their low density high specific strength and high specific stiffness These properties along with better infiltration with reinforcements carbon nanotubes CNTs glass etc capability make them an excellent candidate to fabricate Polymer Matrix Composites PMCs tailored for specific applications The applications range from products used daily to deep space exploration These materials are subjected to varying temperatures and pressures during fabrication and in service Therefore the evolution of their intrinsic properties needs to be studied and their ability to sustain extreme environmental conditions in outer space needs to be investigated Utilizing experimental techniques for this purpose is time consuming and expensive Predictive computational tools like molecular dynamics MD can be used for such studies as they are quick and inexpensive

relative to experiments Furthermore it reduces the overall time in designing and deploying the next generation of composite materials In this work MD is implemented to model self assembled stacks of flattened CNTs flCNTs and polyimide composites to investigate the interfacial properties at the interface between flCNT and polyimides Fluorinated and non fluorinated polyimides are compared based on interaction energy friction force and transverse strength The reactive interface force field IFF R is validated to predict thermo mechanical properties of epoxies for varying degrees of cure These nanoscale properties provide a set of inputs for microscale analysis to predict the evolution of residual stresses for the process modeling of composites In order to use nanoscale mechanical properties as inputs they need to be corrected for the strain rate discrepancy associated with several orders of magnitude difference between experimental and simulated strain rates A phenomenological approach to account for this strain rate difference is developed based on experimental characterization data Once the MD properties are corrected they can be used in microscale analysis to accurately predict residual stresses

**Molecular Modeling of Polymer Solutions Using Brownian Dynamics** Indranil Ghosh,2000 **Molecular Modeling of Intermediate Order in Polymer Glasses** Jon P. Van Order,1999 *Molecular Modeling of Confined Polymers* Owen J. Hehmeyer,2006 Grafted polymers carrying a single charge at the free ends were studied with MC simulation The brush height was found to change substantially with the surface charge density The interaction of the same brush with adsorbing protein was examined with MC and MF It was found that the brush hinders protein adsorption

**Application of Molecular Modeling to Polymer Grafted Nanostructures** ,2004 Polymer chains undergo conformational transitions in response to a change in solvent quality of their environment making them strong candidates to be used in smart nanometer scale devices In the present work molecular modeling is used to explore grafted polymer structures with various functionalities The first part of this research focuses on two examples of selective transport through nanopores modified with polymer brush structures The first is the investigation of solvent flow through nanopores grafted with linear chains Molecular dynamics MD simulations are used to demonstrate how a stretch collapse transition in grafted polymer chains can be used to control solvent flow rate through a nanopore in response to environmental stimuli A continuum fluid dynamics method based on porous layer model for describing flow through the smart nanopore is described and its accuracy is analyzed by comparing with the results from MD simulations The continuum method is then applied to determine regulation of water permeation in response to pH through a poly L glutamic acid grafted nanoporous membrane A second example is use of a rod coil transition in bottle brush molecules that are grafted to the inside of a nanopore to size select macromolecules as they diffuse through the functionalized nanopores These stimuli responsive nanopores have a variety of potential applications including molecular sorting smart drug delivery and ultrafiltration as well as controlled chemical release Tethered polymers play an important role in biological structures as well In the second part of the research application of atomistic simulations to characterize the effect of phosphorylation on neurofilament structure is presented

Neurofilaments are intermediate filaments that regulate axonal diameter through their long flexible side arms extending from the central core Their functionality is imparted by polymer brush like structure that causes steric repulsion between the filament

*Molecular Modeling and Multiscaling Issues for Electronic Material Applications* Nancy Iwamoto,Matthew Yuen,Haibo Fan,2011-12-29 *Molecular Modeling and Multiscaling Issues for Electronic Material Applications* provides a snapshot on the progression of molecular modeling in the electronics industry and how molecular modeling is currently being used to understand material performance to solve relevant issues in this field This book is intended to introduce the reader to the evolving role of molecular modeling especially seen through the eyes of the IEEE community involved in material modeling for electronic applications Part I presents the role that quantum mechanics can play in performance prediction such as properties dependent upon electronic structure but also shows examples how molecular models may be used in performance diagnostics especially when chemistry is part of the performance issue Part II gives examples of large scale atomistic methods in material failure and shows several examples of transitioning between grain boundary simulations on the atomistic level and large scale models including an example of the use of quasi continuum methods that are being used to address multiscaling issues Part III is a more specific look at molecular dynamics in the determination of the thermal conductivity of carbon nanotubes Part IV covers the many aspects of molecular modeling needed to understand the relationship between the molecular structure and mechanical performance of materials Finally Part V discusses the transitional topic of multiscale modeling and recent developments to reach the submicronscale using mesoscale models including examples of direct scaling and parameterization from the atomistic to the coarse grained particle level

*Molecular Modeling of Rigid-Rod Polymers Structures Dominated by Electrostatic Interactions* ,2005 This report results from a contract tasking Institute of Macromolecular Compounds of Russian Academy of Science as follows PBO a rigid rod polymer developed by the Air Force Materials Laboratory and now commercially available from Toyobo has considerable promise for applications as separator membranes in advanced fuel cells and batteries In such applications the performance of the membrane is intimately related to the structure of the polymer In PBO as well as any other polymer used to provide a pathway for ionic conduction electrostatic interactions are likely to play a dominant role in defining that structure PBO is a lyotropic liquid crystalline polymer which is soluble only in very strong acids from which it is processed into fibers or films Electrostatic interactions may play a very large role in their structure formation by virtue of the charged groups on the polymer itself and the small counter ions which accompany them Understanding these interactions may ultimately provide a means of tailoring the morphology which the polymer adopts We propose to undertake a molecular modeling study of the effect of strong acids on the structure and properties of PBO in solution and bulk state by applying the molecular mechanics approach Such studies are necessary before larger scale molecular simulations addressing the physical processes underlying of the development in the processing membranes and fibres of the fibrillar structure can be undertaken Multiscale

Modelling of Polymer Properties E. Perpète, Manuel Laso, 2006-11-18 Modelling in polymer materials science has experienced a dramatic growth in the last two decades Advances in modeling methodologies together with rapid growth in computational power have made it possible to address increasingly complex questions both of a fundamental and of a more applied nature Multiscale Modelling of Polymer Properties assembles research done on modeling of polymeric materials from a hierarchical point of view in which several methods are combined in a multilevel approach to complex polymeric materials Contributions from academic and industrial experts are organized in two parts the first one addresses the methodological aspects while the second one focuses on specific applications The book aims at comprehensively assessing the current state of the field including the strengths and shortcomings of available modelling techniques and at identifying future needs and trends Several levels of approximation to the field of polymer modelling ranging from first principles to purely macroscopic Contributions from both academic and industrial experts with varying fields of expertise Assesses current state of this emerging and rapidly growing field

**Molecular Modeling of Dilute Penetrant Gas Diffusion in a Glassy Polymer Using Multidimensional Transition-state Theory** Michael Lewis Greenfield, 1996

**Tribology of Polymer and Polymer Composites for Industry 4.0** Hemalata Jena, Jitendra Kumar Katiyar, Amar Patnaik, 2021-08-23 This book first introduces polymers and polymer composites which are widely used in different industrial and engineering applications where the proper selection of fiber filler and polymer can be tailored for particular application The primary objective of this book is to broaden the knowledge of tribology of polymer composites in a new dimension for Industry 4.0 For instance the book covers polymer composites used as self lubricating material used in the automotive industry and other manufacturing equipment to reduce the effect of energy loss due to friction and wear This book is of interest to researchers and industrial practitioners who work in the field of tribology of polymer composites manufacturing equipment and production engineering

*Molecular Dynamic Modeling and Simulation for Polymers* Anthony F. Harrell, 2003-09 Polymers have been widely used in various engineering applications For more than a quarter century the materials have been utilized intensively for the binding materials for composites The material properties of the binding materials called matrix materials play an important role for the composite material behaviors As a result the objective of this study was to understand the mechanical properties of polymers In particular the goal was to develop insights as to how a molecular level structure is connected to the bulk properties of materials assuming homogeneity To this end molecular dynamics was used to model and simulate the polymeric behaviors Polymeric chains were modeled using the bead and spring model along with interacting potentials The study examined the effects of different sizes densities and numbers of molecules per chain on the shear moduli of the polymers Furthermore some preliminary study was also conducted for metallic particle reinforced polymer composites

*Application of Molecular Modeling to Polymer Grafted Nanostructures* Shashishekar Parampalli Adiga, 2003 Keywords biopolymers polymer brushes grafted polymers smart nanopores flow control environment responsive nanoporous materials molecular

modeling     Encyclopedia of Polymer Science and Technology, Concise Herman F. Mark, 2013-10-16 The compact affordable reference revised and updated The Encyclopedia of Polymer Science and Technology Concise Third Edition provides the key information from the complete twelve volume Mark's Encyclopedia in an affordable condensed format Completely revised and updated this user friendly desk reference offers quick access to all areas of polymer science including important advances in nanotechnology imaging and analytical techniques controlled polymer architecture biomimetics and more all in one volume Like the twelve volume full edition the Encyclopedia of Polymer Science and Technology Concise Third Edition provides both SI and common units carefully selected key references for each article and hundreds of tables charts figures and graphs     **Foundations of Molecular Modeling and Simulation** Peter T. Cummings, Phillip Ray Westmoreland, Brice Carnahan, 2001

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