

1. Record Nr.	UNINA9910974861303321
Autore	Askadskii A. A (Andrei Aleksandrovich)
Titolo	Computational materials science of polymers // Andrey Aleksandrovich Askadskii
Pubbl/distr/stampa	Cambridge [England], : Cambridge International Science Pub., 2003
ISBN	1-280-22604-8 9786610226047 1-904602-32-0
Descrizione fisica	1 online resource (711 p.)
Disciplina	668.9
Soggetti	Polymers - Mathematical models Plastics
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	PREFACE; INTRODUCTION; Chapter I. Brief information on types of polymers and their chemical structure; Chapter II. Packing of macromolecules and polymer density; II.1. Increments method and basic physical assumptions; II.2. Relationship between free volume of polymers, coefficient of molecular packing and porous structure; Chapter III. Temperature coefficient of volumetric expansion; Chapter IV. Glass transition temperature of polymers; IV.1. Thermomechanical and other methods of evaluation of the glass transition temperature of polymers; IV.2. Mechanism of glass transition IV.3. Calculation of the glass transition temperature of linear polymersIV.4. Influence of plasticization on the glass transition temperature of polymers; IV.5. Calculation of the glass transition temperature of polymer networks; Chapter V. Temperature of transition into the viscous flow state for amorphous polymers; V.1 Estimation of temperature of transition into the viscous flow state of polymers; V.2 Dependence of Newtonian viscosity on molecular mass of polymer in a wide range of its change; Chapter VI. Melting point of polymers Chapter VII. Temperature of onset of intense thermal degradation of polymersChapter VIII. Optical and opto-mechanical properties of polymers; VIII.1 Refractive index; VIII.2 Stress-optical coefficient; Chapter IX. Dielectric constant of polymers and organic solvents;

Chapter X. Equilibrium rubbery modulus for polymer networks; X.1 Calculations of the equilibrium modulus; Chapter XI. Description of relaxation processes in polymers; XI.1 Stress relaxation; XI.2 Sorption and swelling processes; Chapter XII. Solubility of polymers XII.1 Specific cohesive energy of organic liquids and polymers Hildebrand solubility parameter XII.2 Solubility criterion; XII.3 Influence of molecular mass and degree of macromolecule orientation on solubility; Chapter XIII. Surface properties of organic liquids and polymers; XIII.1. Surface tension of organic liquids; XIII.2. Surface tension of polymers; Chapter XIV. Miscibility of polymers; Chapter XVI. Thermophysical properties of polymers; XVI.1 Heat capacity; XVI.2 Thermal diffusivity and heat conductivity
Chapter XVII. Molecular design and computer synthesis of polymers with predetermined properties
Appendix 1. Examples of solution of direct problems of polymer synthesis; Appendix 2. Examples of solving the reverse problem of polymer synthesis; Appendix 3. The example of solving the complex problem ... analysis of the chemical structure of phenol formaldehyde resin; Appendix 4. Application of the approach to multicomponent copolymers; Appendix 5. Influence of strong intermolecular interaction occurring between two dissimilar polymers on their miscibility
Appendix 6. On formation of super-molecular structures in amorphous polymers

Sommario/riassunto

An approach to the quantitative analysis of the effect of the chemical structure of linear and network polymers on their properties is described. The approach is based on the representation of the repeating unit of the polymer in the form of a set of anharmonic oscillators which describe the thermal motion of atoms in the field of intra- and intermolecular forces, including weak dispersion forces, dipole-dipole interactions, hydrogen and valency bonds.
