## **Computational Materials Science of Polymers**



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## Reviews

This type of publication is almost everything and helped me looking forward and much more. I am quite late in start reading this one, but better then never. You wont really feel monotony at whenever you want of your own time (that's what catalogs are for relating to if you ask me). (Prof. Buddy Leuschke)

#### **COMPUTATIONAL MATERIALS SCIENCE OF POLYMERS**



Viva Books Private Limited, 2009. Hardcover. Book Condition: New. First edition. 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. Computer programs based on this approach are also presented. They can be used for calculating more than 50 fundamental physical and chemical constants of linear and network polymers as well as low molecular liquids. The programs make it possible to solve a direct problem, i.e. quantitative evaluation of the physical properties of polymers based on their chemical nature, and a reverse problem, i.e. computer synthesis of polymers with the prescribed physical properties. Contents: Introduction ? Brief information on types of polymers and their chemical structure ? Packing of macromolecules and polymers density ? Increments method and basic physical assumptions ? Relationship between free volume of polymers, coefficient of molecular packing and porous structure ? Temperature coefficient of volumetric expansion ? Glass transition temperature of polymers ? Thermomechanical and other methods of evaluation of the glass transition temperature of polymers ? Mechanism of glass transition ? Calculation of the glass transition temperature of linear polymers ? Influence of plasticization on the glass transition temperature of polymers ? Calculation of the glass transition temperature of polymer networks ? Temperature of transition into the viscous flow state for amorphous polymers ? Estimation of temperature of transition into the viscous flow state of polymers ? Dependence of Newtonian viscosity on molecular mass of polymer in a wide range of its change ?...

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