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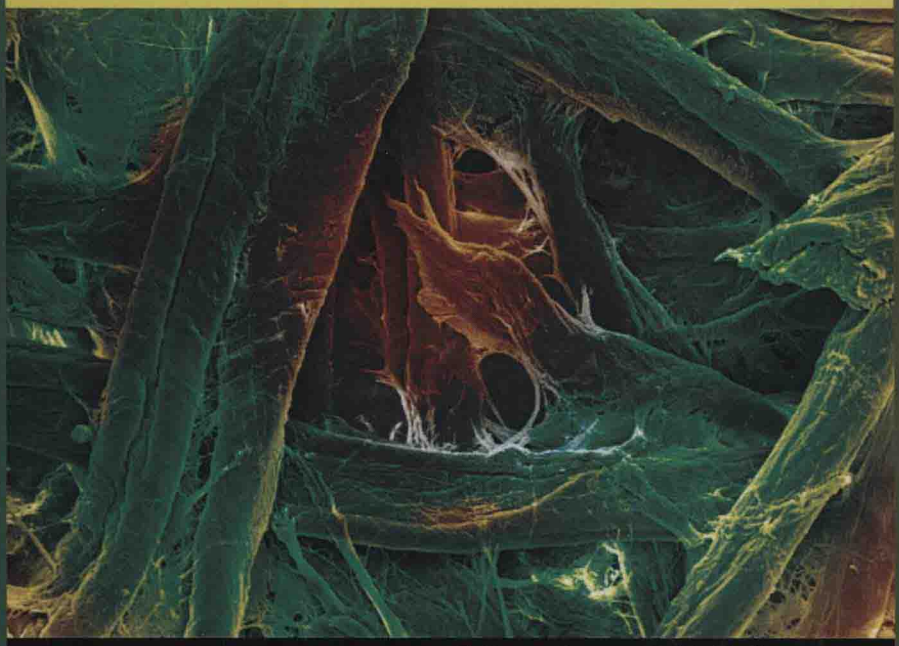
Key Research and Development



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LIST OF ABBREVIATIONS

AFM	atomic-force microscope
BD	Brownian dynamics
CHC	Cahn–Hilliard–Cook
CNTs	carbon nanotube's
DFT	dynamic density functional theory
DGEBA	diglycidyl ether of bisphenol-A
DMTA	dynamic mechanical thermal analyzer
DPD	dissipative particle dynamics
ERM	effective reinforcing modulus
FEM	finite element method
HA	hexylamine
HMDA	hexamethylenediamine
LB	lattice Boltzmann
MC	Monte Carlo
MD	molecular dynamics
MM	molecular mechanics
MWCNTs	multiwalled CNTs
PMMA	poly(methyl methacrylate)
RVE	representative volume element
SUSHI	Simulation Utilities for Soft and Hard Interfaces
SWCNTs	single-walled CNTs
TDGL	time-dependent Ginsburg–Landau

PREFACE

This book facilitates the study of problematic chemicals in such applications as chemical fate modeling, chemical process design, and experimental design. This volume provides comprehensive coverage of modern physical chemistry and chemical engineering.

In the first chapter, aiming to control by stress birefringence the radiotransparent fiber-glass plastic products based on highly cross-linked polymer matrices, theoretical regularities for mathematical description of this property were developed. Computer physical modeling of topological structure of experimental objects was carried out on epoxy-amine polymers with different cross-link density taken as an example. And constants of this model were specified. The adequacy of the model was demonstrated by comparison of the model-calculated against experimental approach to thermal polarization curves.

Hyaluronan (HA) is a high-molecular weight, naturally occurring linear polysaccharide and found in all tissues and body fluids of higher animals. The excellent properties of HA such as biodegradability, biocompatibility, safety, excellent mucoadhesive capacity and high water retaining ability make it well-qualified for using in various bio-medical applications. In addition, HA is nontoxic, noninflammatory, and nonimmunogenic. Because of all these advantages, HA has received much attention as a matrix for drug delivery system. Chapter 2 will summarize our present knowledge about HA, as well as its properties and its development in some pharmaceutical applications.

The goal of Chapter 3 is to review the adhesive bonding of steel sheets treated by nitrooxidation and to compare the acquired results to the nontreated steel.

In Chapter 4, for the first time in the world practice the results of simulation by the Monte Carlo method of the kinetics of three-dimensional free-radical polymerization of tetrafunctional monomers (TFM) were obtained in the framework of the formation of a unitary three-dimensional structural element (UTDSE) and their structure formation on the simple

cubic lattice, depending on the length l of molecules tetrafunctional monomers (l = 1 to 40 ribs of the lattice). Peculiarities of kinetics of changes in parameters such as the degree of polymerization of the Pn UTDSE, the number of radicals, the number of cross-links and cycles, and other characteristics were revealed. It was established that UTDSE are characterized by low levels of P_n for l = 1 and an explanation of this phenomenon was given. The study of the granulometric distribution (GMD) of UTDSE showed that curves of GMDs are bimodal and the probability density of these maximums was calculated.

The research in Chapter 5 is devoted to creation of elastomeric compositions based on systems with functionally active components for extreme conditions. The use of polycondensation capable monomers (PCCM) and other compounds with reactive groups was proposed for generating the stabilizing physical and chemical transformations. Thermodynamic analysis of open polycondensation systems and substantiation of various PCCM application as functionally active components of elastomeric materials have been conducted in the work; research results of polycondensation in an elastomeric matrix have been represented and a possibility of improving heat and corrosion resistance of elastomeric materials with introduction PCCM has been shown; and different ways of applying PCCM have been proposed and experimentally proved.

Aromatic polyimides and polyamides-based 4,4′-diaminothreephenylmethane has been synthesized. Their thermal, rheological properties and solubility in various organic solvents have been studied. In Chapter 6, it is shown that the solubility of the obtained polymers is connected with a free internal rotation triphenylmethan of bridge group and an effect of a surround phenyl substituent in diaminodiphenylmethane.

Possibilities of utilization of biopolymers, and particularly of the deoxyribonucleic acid (DNA) are reviewed and discussed in Chapter 7. The ways of their functionalization with photoresponsive molecules to get desired properties are described and illustrated on several examples as well as the processing of materials into thin films. Their room – and photothermal stability, studied by spectroscopic techniques is reported, together with optical damage thresholds. Physical properties and, more particularly linear, nonlinear and photoluminescent properties of obtained materials are also reviewed and discussed.

In Chapter 8, NMR ^{1}H and ^{13}C spectra of *tert*-butyl hydroperoxide in acetonitrile-d_3, chloroform-d and dimethyl sulfoxide-d_6 have been investigated by the NMR method. The calculation of magnetic shielding tensors and chemical shifts for ^{1}H and ^{13}C nuclei of the *tert*-butyl hydroperoxide molecule in the approximation of an isolated particle and considering the influence of the solvent in the framework of the continuum polarization model was carried out. Comparative analysis of experimental and computer NMR spectroscopy results revealed that the GIAO method with MP2/6–31G (d,p) level of theory and the PCM approach can be used to estimate the parameters of NMR ^{1}H and ^{13}C spectra of *tert*-butyl hydroperoxide.

Air pollution source by manufacture of ceramic materials are emissions of a smoke from refire kilns. Designs on modernization of system of an aspiration of smoke fumes of refire kilns in manufacture ceramic and refractories are devised. In this regard, experimental researches of efficiency of clearing of gas emissions are executed in Chapter 9. Modelling of process of a current of a gas-liquid stream is implemented in the program of computing hydrodynamics Ansys CFX. The ecological result of implementation of system consists highly clearings of a waste-heat and betterment of ecological circumstances in a zone of the factories.

In Chapter 10, an update on the modeling and mechanical properties of CNT/polymer nano-composites is presented. A very comprehensive references and further reading is also provided at the end of this chapter as well. Chapter 11 provides a detailed review on relevant approach of 3D reconstruction from two views of single 2D image and it potential applications in pore analysis of electrospun nanofibrous membrane. The review has concisely demonstrated that 3D reconstruction consists of three steps which is equivalent to the estimation of a specific geometry group. These steps include: estimation of the epipolar geometry existing between the stereo image pair, estimation of the affine geometry, and also camera calibration. The advantage of this system is that the 2D images do not need to be calibrated in order to obtain a reconstruction. Results for both the camera calibration and reconstruction are presented to verify that it is possible to obtain a 3D model directly from features in the images. Finally, the applications of 3D reconstruction in pore structure characterization of electrospun nanofibrous membrane are discussed.

Today, energy is an important requirement for both industrial and daily life, as well as political, economical, and military issues between countries. While the energy demand is constantly increasing every day, existing energy resources are limited and slowly coming to an end. Due to all of these conditions, researchers are directed to develop new energy sources which are abundant, inexpensive, and environmentally friendly. The solar cells, which directly convert sunlight into electrical energy, can meet these needs of mankind. Chapter 12 reviews the efforts in incorporating of solar cells into textile materials.

Quantum-chemical calculation of molecules dekacene, eicocene was done by method MNDO in Chapter 13. And optimized by all parameters geometric and electronic structures of these compounds. Each of these molecular models has a universal factor of acidity equal to 33 (pKa=33). They all pertain to class of very weak H-acids (pKa>14).

In Chapter 14 ceramization (ceramification) of polymer composites is presented as a promising method for gaining flame retardancy of the materials. Because of its passive fire protecting character, ceramization effect can be applied in polymer composites, which are dedicated for work in public places like shopping centers, sport halls, galleries and museums, office buildings, theaters or cinemas and public means of transport. In case of fire, ceramizable polymer composites turn into barrier ceramic materials, ensuring integrity of objects like electrical cables, window frames, doors, ceilings, etc., exposed on flames and heat, preventing from collapsing of materials and making electricity working, enabling effective evacuation. Moreover, ceramization process decreases emission of toxic or harmful gaseous products of polymer matrix degradation as well as its smoke intensity. The chapter describes mechanisms of ceramization for various polymer composites, especially focusing on silicone rubber-based ones, basic characteristics of the materials and ways of their testing.

In Chapter 15, we have attempted to establish relationships between the phase viscosity ratios of liquid gelatin (2%)-LBG (0.8%) systems and their rheological properties. To do that, LBG samples with different degrees of thermodegradation were taken.

In Chapter 16, a kinetic method of analysis of compounds from edible and medicinal plant extracts activity against stable radical 2,2-diphenyl-1-picrylhydrazyl (DPPH) is developed. The initial rate of DPPH's decay

in standard conditions is suggested and theoretically explained as a kinetic parameter to compare the extract antiradical activity. A 10–150-fold decrease of the DPPH's reaction rate with plant extract antioxidants is achieved by the addition of acids into the reaction medium. Such results were explained by changes of input of different mechanisms into the whole process of scavenge of DPPH radical. A decrease of the reaction rate for the optimum of added acid's concentration with the acid strength increasing is also observed. The influence of the acids extracted from plant material on the results is excluded by this method because of the stronger acid addition. It is found that the linear interval of the dependence of DPPH's conversion degree after the first 30 min from the start of the reaction vs. the initial antioxidant concentration lies from 0 to 60%.

Chapter 17 discusses the development of a mathematical model for describing stress birefringence of highly cross-linked polymer matrices. Chapter 18 of this book gives an update on modern fibers, fabrics, and clothing.

This book offers a valuable overview and myriad details on current chemical processes, products, and practices. The book serves a spectrum of individuals, from those who are directly involved in the chemical industry to others in related industries and activities. It provides not only the underlying science and technology for important industry sectors, but also broad coverage of critical supporting topics.