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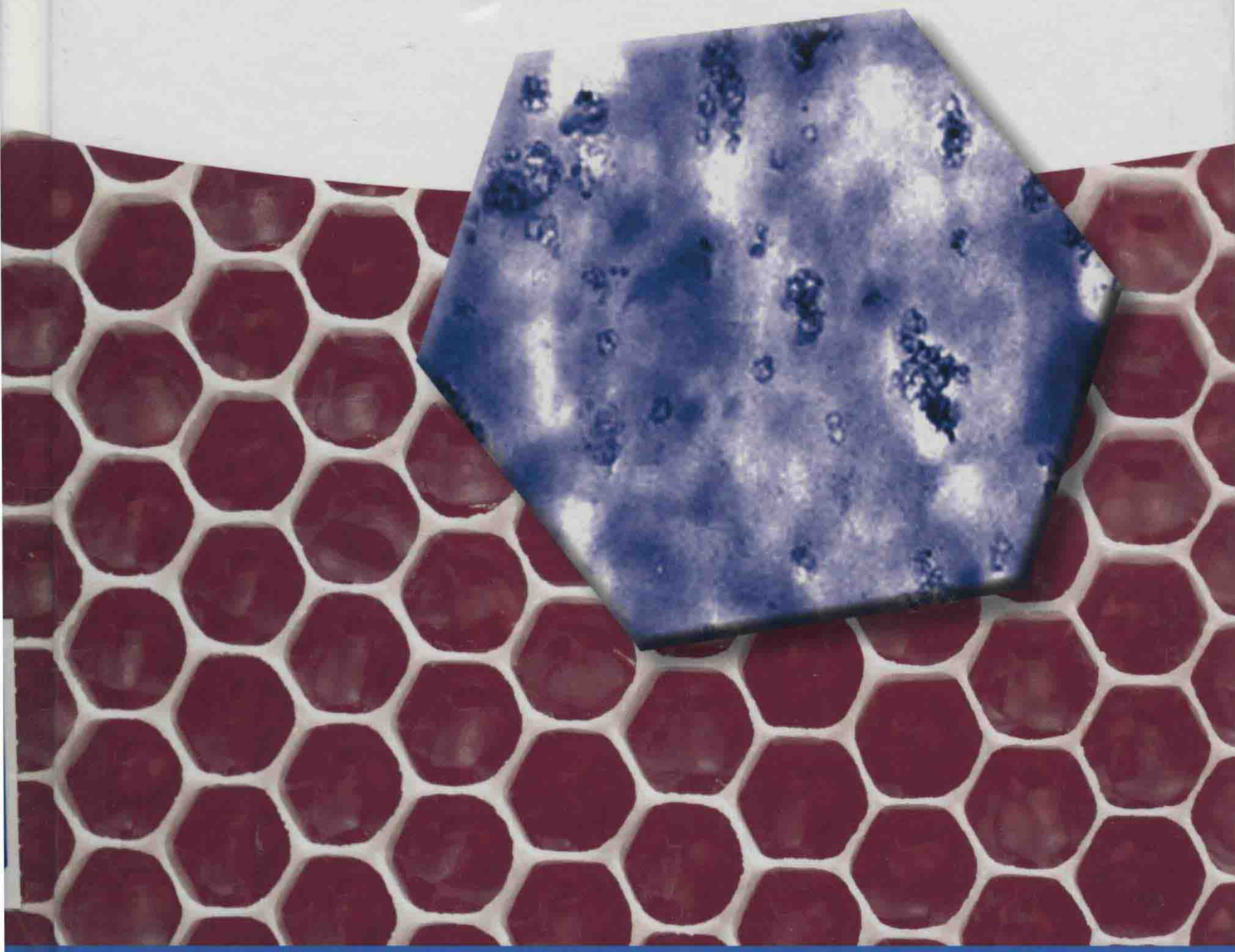
Modeling and Prediction of Polymer Nanocomposite Properties



Polymer Nano-, Micro- & Macrocomposites

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Preface

Modeling and prediction of the nanocomposite properties is generally achieved using different finite element, statistical and micromechanical models. These models help in predicting the properties of the nanomaterials, thus eliminating the need for synthesizing each and every composite first to ascertain its properties. A number of precautions are, however, necessary in order to avoid discrepancies in the model outcome, for example, the model used should not have unrealistic assumptions and the experimental results should be in plenty in order to have an accurate model. The validation of the model should also be achieved by a comparison of the predicted values with the experimental values. The chapters contained in the book present examples of modeling and prediction of polymer clay nanocomposite properties using various types of theoretical methods.

Chapter 1 comments on the convergence of the experimental and theoretical studies and reviews briefly the various kinds of melds used for the prediction of nanocomposite properties. Chapter 2 reviews the application of Self-Consistent Field Theory (SCFT) to prediction of polymer-clay nanocomposite morphology. Over the past decade, SCFT has been shown to qualitatively describe the factors influencing the polymer ability to intercalate or exfoliate the clay platelets. In Chapter 3, the experimental analysis of particulate-filled nanocomposites butadiene-styrene rubber/fullerene-containing mineral (nanoshungite) is analyzed with the aid of force-atomic microscopy, nanoindentation methods, and computer treatment. The theoretical analysis is carried out within the frameworks of fractal analysis. Chapter 4 presents a reptation-based model that incorporates polymer-particle interactions and confinement to describe the dynamics and rheological behaviors of linear entangled polymers filled with isotropic nanoscale particles. In Chapter 5, a hierarchical procedure for bridging the gap between atomistic and macroscopic modeling via mesoscopic simulations is presented. The concept of multiscale modeling is outlined, and relevant examples of applications of single scale and multiscale procedures for nanostructured systems of industrial interest are illustrated. The behavior of polymer-layered silicate nanocomposites is modeled in Chapter 6 through various factorial and mixtures design methodologies in order to optimize the composite performance and to accurately predict the properties especially for the non-polar polymer systems. Chapter 7 introduces a hierarchical multiscale and stochastic Finite Element Method (MSFEM) to model the spatial randomness induced in polymers by the non-uniform distribution of nanophases including primarily single walled carbon nanotubes (SWCNT). In Chapter 8, a general effective medium model derived from "grain averaging theory"—in analogy to quantum scattering theory—is reviewed in which anisotropicity of the second phase (filler from hereafter) can be included. Chapter 9 presents a new technique that takes into account the curvature that the nanotubes show when immersed in the polymer, and is based on a numerical-analytical approach that has significant advances over micromechanical modeling and can be applied to several kinds of nanostructured composites. In Chapter 10, details of the coarse grain scheme from molecular dynamics (MD) to dissipative particle dynamics (DPD) modeling are discussed. Two polymer nanocomposite case studies – PE/PLLA (polyethylene/poly lactic acid) and PE/PLLA/CNT – are provided to demonstrate how multiscale simulation can describe the effects of volume fraction and mixing method on the structure. Chapter 11 presents a product design approach and strategy to design wheat straw polypropylene composites (WSPPC). In this approach, a product design problem is connected to and simultaneously solved with process-product problem to create new products that satisfy the market needs. In Chapter 12, a *kinetic model* is used to predict the reaction rate and the degree of cure as a function of time and temperature; whereas a *rheological model* describes viscosity as a function of time and temperature. Since viscosity is also dependent on the degree of cure, the rheological model combined with the kinetic model forms a *chemorheological model*.

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Contents