

Structure-Property Correlations in Model Composite Materials

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We investigate the effective properties (conductivity, diffusivity and elastic moduli) of model random composite media derived from Gaussian random fields and overlapping hollow spheres. The morphologies generated in the models exhibit low percolation thresholds and give a realistic representation of the complex microstructure observed in many classes of composites. The statistical correlation functions of the models are derived and used to evaluate rigorous bounds on each property. Simulation of the effective conductivity is used to demonstrate the applicability of the bounds. The key morphological features which effect composite properties are discussed.

I. INTRODUCTION

The prediction of effective properties of heterogeneous systems such as porous media and two phase composites is of considerable interest [1-3]. Understanding the inter-relationships between rock properties and their expression in geophysical and petrophysical data is necessary for enhanced characterisation of underground reservoirs. This understanding is crucial to the economics of oil and gas recovery, geothermal energy extraction and groundwater pollution abatement. Manufactured composites such as foamed solids [4] and polymer blends [5] often exhibit a complex microstructure. To optimize the properties of these systems it is necessary to understand how morphology influences effective properties. In general, the difficulty of accounting for microstructure has made exact prediction impossible in all but the simplest of cases.

On the other hand, considerable progress has been made in the derivation of rigorous bounds on a host of properties [1,6]. For example, relatively accurate bounds have been derived for the elastic moduli and conductivity of isotropic two-phase composites [7-11]. To evaluate these bounds for a given system it is necessary to know

the 3-point statistical correlation function [12]. Due to the difficulty of measuring this information [13-15], a number of model media have been proposed for which the functions can be explicitly evaluated. These include: cellular [16], particulate [1] and periodic [17] materials (eg. Figs. 1(a)&(b)). The principal problem with these models is that they employ over-simplified representations of the inclusion (or pore) structure observed in many natural and manufactured composite materials.

Recently we derived the properties of a model of amorphous materials [18] (eg. Fig. 1(c)) based on level-cut Gaussian random fields [19] (GRF). Although the GRF model is applicable to many classes of non-particulate composite materials, it cannot account for materials which remain percolative at very low volume fractions.

Porous rocks [3,20], polymer blends [5], solid foams [4] and membranes provide examples of systems where a single phase remains connected down to low volume fractions. The percolation threshold of a system is only one factor which determines its effective properties: The shape of the pores/inclusions should also be considered [21-23]. Polystyrene foam, an example of a highly-porous material, is shown in Fig. 2.

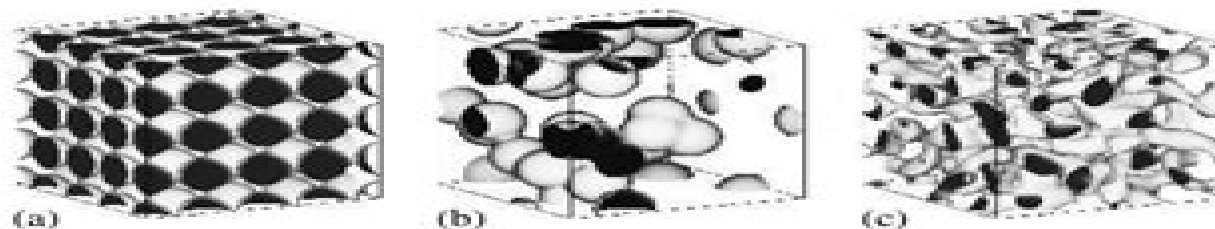


FIG. 1. Models of composite microstructure. (a) Periodic models - regular array of spheres; (b) Particulate models - identical overlapping spheres (IOS) and; (c) Gaussian random field (GRF) models - single-cut variant. None of the models can mimic the microstructure observed in percolative low volume fraction materials (eg. polystyrene foam - Fig. 2).

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Structure Property Correlations In Drug Research

Mark T.D. Cronin



Structure Property Correlations In Drug Research:

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Pharmaceutical Sciences: Breakthroughs in Research and Practice Management Association, Information Resources, 2016-12-28 The delivery of optimal pharmaceutical services to patients is a pivotal concern in the healthcare field By examining current trends and techniques in the industry processes can be maintained and improved Pharmaceutical Sciences Breakthroughs in Research and Practice provides comprehensive coverage of the latest innovations

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Methods of Drug Discovery Alexander Hillisch,Rolf Hilgenfeld,2012-11-28 Research in the pharmaceutical industry today is in many respects quite different from what it used to be only fifteen years ago There have been dramatic changes in approaches for identifying new chemical entities with a desired biological activity While chemical modification of existing leads was the most important approach in the 1970s and 1980s high throughput screening and structure based design are now major players among a multitude of methods used in drug discovery Quite often companies favor one of these relatively new approaches over the other e g screening over rational design or vice versa but we believe that an intelligent and concerted use of several or all methods currently available to drug discovery will be more successful in the medium term What has changed most significantly in the past few years is the time available for identifying new chemical entities Because of the high costs of drug discovery projects pressure for maximum success in the shortest possible time is higher than ever In addition the multidisciplinary character of the field is much more pronounced today than it used to be As a consequence researchers and project managers in the pharmaceutical industry should have a solid knowledge of the more important methods available to drug discovery because it is the rapidly and intelligently combined use of these which will determine the success or failure of preclinical projects **Smith and Williams' Introduction to the Principles of Drug Design and Action** H. Jphn Smith,H. Jphn Williams,2005-10-10

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Predicting Chemical Toxicity and Fate Mark T.D. Cronin, 2004-05-10 Quantitative Structure Activity Relationships QSARs are increasingly used to predict the harmful effects of chemicals to humans and the environment The increased use of these methods in a variety of areas academic industrial regulatory results from a realization that very little toxicological or fate data is available on the vast amount of chemicals to which humans and the environment are exposed Predicting Chemical Toxicity and Fate provides a comprehensive explanation of the state of the art methods that are available to predict the effects of chemicals on humans and the environment It describes the use of predictive methods to estimate the physiochemical properties biological activities and fate of chemicals The methods described may be used to predict the properties of drugs before their development and to predict the environmental effects of chemicals These methods also reduce the cost of product development and the need for animal testing This book fills an obvious need by providing a comprehensive explanation of these prediction methods It is a practical book that illustrates the use of these techniques in real life scenarios This book will demystify QSARs for those students unsure of them and professionals in environmental toxicology and chemistry will find this a useful reference in their everyday working lives

Chemoinformatics for Drug Discovery Jürgen Bajorath, 2013-11-18 Chemoinformatics strategies to improve drug discovery results With contributions from leading researchers in academia and the pharmaceutical industry as well as experts from the software industry this book explains how chemoinformatics enhances drug discovery and pharmaceutical research efforts describing what works and what doesn't Strong emphasis is put on tested and proven practical applications with plenty of case studies detailing the development and implementation of chemoinformatics methods to support successful drug discovery efforts Many of these case studies depict groundbreaking collaborations between academia and the pharmaceutical industry Chemoinformatics for Drug Discovery is logically organized offering readers a solid base in methods and models and advancing to drug discovery applications and the design of chemoinformatics infrastructures The book features 15 chapters including What are our models really telling us A practical tutorial on avoiding common mistakes when building predictive models Exploration of structure activity relationships and transfer of key elements in lead optimization Collaborations between academia and pharma Applications of chemoinformatics in pharmaceutical research experiences at large international pharmaceutical companies Lessons learned from 30 years of developing successful integrated chemoinformatic systems Throughout the book the authors present chemoinformatics strategies and methods that have been proven to work in pharmaceutical research offering insights culled from their own investigations Each chapter is extensively referenced with citations to original research reports and reviews

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