

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 optimise 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 (e.g. 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] (e.g. 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.

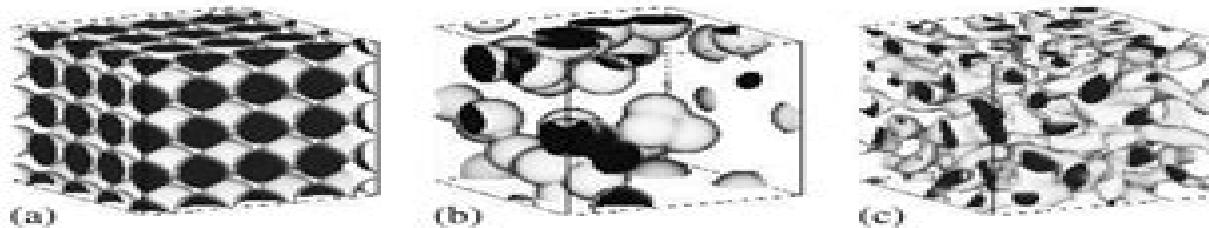


FIG. 1. Models of composite microstructure. (a) Periodic models - regular array of spheres; (b) Particulate models - identical overlapping spheres (MOS); and; (c) Gaussian random field (GRF) models - single cut variant. None of the models can mimic the microstructure observed in percolative low volume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

Structure Property Correlations In Drug Research

Roberto Todeschini, Viviana Consonni

Structure Property Correlations In Drug Research:

Structure-property Correlations in Drug Research Han van de Waterbeemd, 1996 This book provides an overview of statistical chemometric methods used in the rapidly changing arena of drug discovery. It deals with physicochemical molecular descriptors, modern statistical methods to study structure property and structure activity relationships including three dimensional QSAR approaches and the concepts of molecular diversity. All scientists who investigate quantitative structure activity relationships in medicinal, agricultural or environmental chemistry should benefit from this book.

Handbook of Molecular Descriptors Roberto Todeschini, Viviana Consonni, 2008-07-11 Quantitative studies on structure activity and structure property relationships are powerful tools in directed drug research. In recent years various strategies have been developed to characterize and classify structural patterns by means of molecular descriptors. It has become possible not only to assess diversities or similarities of structure databases but molecular descriptors also facilitate the identification of potential bioactive molecules from the rapidly increasing number of compound libraries. They even allow for a controlled de novo design of new lead structures. This is the most comprehensive collection of molecular descriptors and presents a detailed review from the origins of this research field up to present day. This practically oriented reference book gives a thorough overview of the different molecular descriptors representations and their corresponding molecular descriptors. All descriptors are listed with their definition, symbols and labels, formulas, some numerical examples, data and molecular graphs while numerous figures and tables aid comprehension of the definitions. Cross references throughout a list of acronyms and notations allow easy access to the information needed to solve a specific research problem. Examples of descriptor calculations along with tables of descriptor values for a set of selected reference compounds and an up to date reference list add to the practical value of the book, making it an invaluable guide for all those dealing with bioactive molecules as well as for researchers.

Molecular Descriptors for Chemoinformatics Roberto Todeschini, Viviana Consonni, 2009-10-30 The number one reference on the topic now contains a wealth of new data. The entire relevant literature over the past six years has been painstakingly surveyed resulting in hundreds of new descriptors being added to the list and some 3 000 new references in the bibliography section. Volume 1 contains an alphabetical listing of more than 3300 descriptors and related terms for chemoinformatic analysis of chemical compound properties while the second volume lists over 6 000 references selected from 450 journals. To make the data even more accessible the introductory section has been completely re-written and now contains several walk-through reading lists of selected keywords for novice users.

Combinatorial Library Design and Evaluation Arup Ghose, Vellerkad Viswanadhan, 2001-06-26 This text traces developments in rational drug discovery and combinatorial library design with contributions from 50 leading scientists in academia and industry who offer coverage of basic principles, design strategies, methodologies, software tools and algorithms and applications. It outlines the fundamentals of pharmacophore modelling and 3D Quantitative Structure Activity

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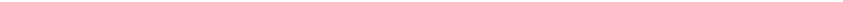
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