

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.

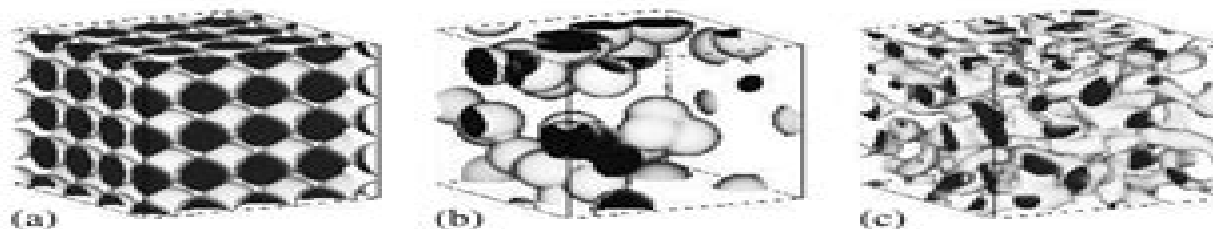


FIG. 1. Models of composite microstructure. (a) Periodic models - regular array of spheres; (b) Particulate models - identical overlapping spheres (IOS) and; (c) Gaussian random field (GRF) models - single-cut variant. None of the models can mimic the microstructure observed in percolative low volume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

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Structure Property Correlations In Drug Research

Roberto Todeschini, Viviana Consonni



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drug discovery process from conception of the molecules to drug production Updated chapters devoted to the discovery of new lead compounds including combinatorial chemistry **Genome Mapping in Plants** Andrew H. Paterson,1996 **3D QSAR in Drug Design** Hugo Kubinyi,Gerd Folkers,Yvonne Connolly Martin,1998 *Particle Bombardment for Genetic Engineering of Plants* Paul Christou,1996-08-02 Particle bombardment is an effective method for introgressing foreign genes into varieties of cultivated crops and has now been established as the method of choice for the engineering of plant species which until recently were viewed as unlikely candidates for genetic manipulation This book brings together all that is known about the technique and provides a comprehensive review of principles and applications of particle bombardment Includes a thorough Introduction to topic Describes the most common bombardment techniques currently in use Provides specific examples to give the reader an appreciation of each bombardment technique Covers numerous model systems including legumes cereals woody species ornamentals oilseed crops and fiber species *Medicinal Chemistry* Frank D. King,2002 This book introduces the principles and practices of modern medicinal chemistry and covers all aspects of drug discovery from the initial lead to final development It teaches how to convert a lead compound into a potential drug and provides recent case histories as examples of successes Medicinal Chemistry is unique in dealing with the subject in such a practical way and is the only book currently available to bring together all areas of the subject in one volume This breadth of coverage is supplemented by references to specialist monographs and reviews where the reader can find more detail on specific topics of interest if required Medicinal Chemistry is essential reading for students studying medicinal chemistry as it provides a grounding in all the required disciplines and subjects It will also be of great interest to chemists biochemists and pharmacologists either already working in or contemplating a career in the pharmaceutical and allied industries

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