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# Measures of microstructure to improve estimates and bounds on elastic constants and transport coefficients in heterogeneous media

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**Abstract**

The most commonly discussed measures of microstructure in composite materials are the spatial correlation functions, which in a porous medium measure either the grain-to-grain correlations, or the pore-to-pore correlations in space. Improved bounds based on this information such as the Beran–Molyneux bounds for bulk modulus and the Beran bounds for conductivity are well-known. It is first shown how to make direct use of bounds and spatial correlation information to provide estimates that always lie between these upper and lower bounds for any microstructure whenever the microgeometry parameters are known. Then comparisons are made between these estimates, the bounds, and two new types of estimates. One new estimate for elastic constants makes use of the Peselnick–Meister bounds (based on Hashin–Shtrikman methods) for random polycrystals of laminates to generate self-consistent values that always lie between the bounds. A second new type of estimate for conductivity assumes that measurements of formation factors (of which there are at least two distinct types in porous media, associated respectively with pores and grains for either electrical and thermal conductivity) are available, and computes new bounds based on this information. The paper compares and contrasts these various methods in order to clarify just what microstructural information—and how accurately that information—needs to be known in order to be useful for estimating material constants in random and heterogeneous media.


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## 1. Introduction

A wide array of results is available for practical studies of linear elastic constants of composite solid and/or granular materials, fluid suspensions, and emulsions. These results range from rigorous bounds such as the Voigt (1928), Reuss (1929), Hill (1952), and Hashin and Shtrikman (1962, 1963a,b) bounds to the fairly popular and mostly well-justified [for sufficiently small concentrations of inclusions (Berryman and Berge, 1996)] approximate methods such as the explicit approximations of Kuster and Toksöz (1974) and Mori and Tanaka (Benveniste, 1987;

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Ferrari and Filiponni, 1991) and the implicit methods such as the differential effective medium (DEM) method (Cleary et al., 1980; Norris, 1985) and the self-consistent (Hill, 1965; Budiansky, 1965), or the coherent potential approximation (CPA) for elastic composites (Gubernatis and Krumhansl, 1975; Korringa et al., 1979; Berryman, 1980a,b, 1982). Older reviews (Watt et al., 1976) and both early (Hashin, 1962; Beran, 1968; Christensen, 1979) and more recent textbooks and research monographs (Mura, 1987; Nemat-Nasser and Hori, 1993; Cherkaev, 2000; Milton, 2002; Torquato, 2002) survey the state of the art. So it might seem that there is little left to be done in this area of research.

However, continuing problems with applications of these methods have included: (a) lack of sufficient microstructural information [such as the commonly required spatial correlation functions (Torquato, 1980, 1982; Berryman, 1985a,b)] needed to compute some of the most accurate bounds known and (b) the failure of some of the explicit methods to satisfy the rigorous bounds in some limiting cases such as three or more constituents (Norris, 1989) or extreme geometries such as disk-like inclusions (Berryman, 1980b). The best implicit schemes—even though they are known to be realizable and, therefore, cannot ever violate the bounds—are often criticized by some workers (Christensen, 1990) because the inherent microgeometry generated automatically by these methods does not represent the details of the true microgeometry with any obvious fidelity. Nevertheless, it has been shown (Berge et al., 1993, 1995) that knowing general features of the microgeometry such as whether one constituent can be classified as the host medium and others as inclusions, or whether in fact there is no single constituent that serves as the host can be sufficient information in itself to decide on a model that can then be used successfully to study an appropriate class of composites (Berge et al., 1993, 1995; Berryman and Berge, 1996; Garboczi and Berryman, 2000, 2001). Some critics also point out that the iteration or integration schemes required to compute the estimates for implicit schemes are sufficiently more difficult to implement than those of the explicit methods that workers are often discouraged from trying these approaches for this reason alone.

Virtually all of the improved bounds (i.e., those providing tighter estimates than the now standard bounds of Hashin and Shtrikman, which typically do not make direct use of microstructural information except for the volume fractions) require some information about the microstructure. But it has not been very clear just how accurately this information needs to be known in order for it to be useful. The present work will show for several examples that some general knowledge of microstructure can be used in several different ways to generate estimates. And since the predicted properties (at least in some cases) do not seem to depend too strongly on details beyond those readily incorporated, it gives some confidence that the methods can be successfully applied to real materials. One comparison we make is between bounds and estimates on elastic constants for random polycrystals of laminates (Berryman, 2004b, 2005b) and the improved bounds and estimates based on spatial correlation functions for disk-like inclusions. Although it is clear physically that these models should both apply at least approximately to the same types of random composites for some ranges of volume fractions, nevertheless the assumed microstructure is organized rather differently in these two cases. The random polycrystal is an aggregate of grains, each of which is a laminate material. These laminated grains are then jumbled together with random orientations—so the overall composite is isotropic, even though the individual grains act like crystals having hexagonal symmetry. For comparison, composites with disk-shaped inclusions must have a microstructure that is at least crudely the same as the random polycrystal, since each layer of an individual grain could be seen as approximately disk-like. So one quantitative question we can ask is: How closely do these two models agree with each other, and if they are indeed close in value, what do we learn about the sensitivity of elastic constants to microstructure? Also, we might ask: How does this information affect engineering efforts towards design (Cherkaev, 2000; Torquato et al., 2003) of new materials?

Section 2 addresses these questions for elastic constants. Section 3 treats similar questions for electrical conductivity and related material constants such as dielectric constant, thermal conductivity, and fluid permeability. Numerical examples are included in both sections. The final section provides some discussion and our overall assessment and conclusions.

## 2. Elasticity: canonical functions and the *Y*-transform

### 2.1. Canonical functions $\Lambda$ and $\Gamma$

To make progress towards our stated goals, it will prove helpful to take advantage of some