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The influence of two-point statistics on the Hashin–Shtrikman bounds for three phase composites[☆]

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ABSTRACT

In this work we analyse the influence of the spatial distribution function, introduced by Ponte Castañeda and Willis (1995), on the Hashin–Shtrikman bounds on the effective transport properties of a transversely isotropic (TI) three-phase particulate composite, i.e. when two distinct materials are embedded in a matrix medium. We provide a straightforward mechanism to construct associated bounds, independently accounting for the shape, size and spatial distribution of the respective phases, and assuming ellipsoidal symmetry.

The main novelty in the present scheme resides in the consideration of more than a single inclusion phase type. Indeed, unlike the two-phase case, a two-point correlation function is necessary to characterize the spatial distribution of the inclusion phases in order to avoid overlap between different phase types. Moreover, once the interaction between two different phases is described, the scheme developed can straightforwardly be extended to multiphase composites.

The uniform expression for the associated Hill tensors and the use of a proper tensor basis set, leads to an explicit set of equations for the bounds. This permits its application to a wide variety of phenomena governed by Laplace's operator. Some numerical implementations are provided to validate the effectiveness of the scheme by comparing the predictions with available experimental data and other theoretical results.

1. Introduction

The prediction of the effective transport and elastic properties of multiphase materials has attracted the attention of scientists and engineers over many years now. Such materials, whether they be naturally occurring or synthetic, frequently exhibit enhanced physical and mechanical properties. The determination of such macroscopic or *effective* properties of reinforced materials, polymers, biomaterials and the exploration of the nature of hydrocarbon reservoirs are just a few of the many applications. From a mathematical point of view, the exact prediction of the effective properties of media characterized by a microstructure is generally an impossible assignment, since the associated physical phenomena are governed by partial differential equations with rapidly varying coefficients.

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Before the early sixties, key results were given by Wiener [1] in 1912 for the effective conductivity and Voigt [2] and Reuss [3] in 1889 and 1928 respectively, in the case of elastic modulus tensor. These latter results were identified as upper and lower *bounds* ($\mathbf{C}^R \le \mathbf{C}^* \le \mathbf{C}^V$) on the effective elastic properties $\mathbf{C}^*$, and for a composite whose rth constituent modulus is labelled $\mathbf{C}^r$, $r = 0, \ldots, n$ they are

$$\mathbf{C}^V = \sum_{r=0}^{n} \xi_r \mathbf{C}^r, \qquad \mathbf{C}^R = \left(\sum_{r=0}^{n} \xi_r (\mathbf{C}^r)^{-1} \right)^{-1}, \qquad \xi_r\text{: } r\text{th phase volume fraction.}$$

Wiener's results provided the same form of bounds but for the transport scenario. The rapid development of the aerospace industry initiated numerous contributions to the subject in the early sixties; especially as regards the understanding of the overall behaviour of more complicated geometries such as fibre-reinforced composites. In particular Hashin and Shtrikman [4] established a variational principle for elastostatics which they subsequently applied to multiphase (macroscopically isotropic) composites [5] and the resulting bounds have become known as the *Hashin–Shtrikman* (HS) bounds on multiphase media. The advantage of the HS bounds over the Reuss–Voigt bounds is that the former use information about the macroscopic anisotropy of the composite, and thus permit an improvement over the Reuss–Voigt bounds in almost all cases. Derivations of the HS bounds have been improved by many authors since they were originally devised, see e.g. [6,7] and for a recent exposition of the nature of their construction [8].

Of particular note is the work by Ponte-Castañeda & Willis [9], who introduced a comparison material and included additional microstructural information represented by a two-point correlation function. This permitted the derivation of a more general methodology for n distinct types of inclusion phases that could be selected independently of their spatial distribution, although their applications were all associated with two phase materials. Indeed over the last few decades, although a large number of approaches have been proposed to predict the effective properties for the two phase case (see e.g. [1,3,10,11,2,12]), the three-phase model (of special significance in the effective thermal conductivity of unsaturated soils for example) has been treated less frequently. Amongst the authors who have treated such problems is the composite spheres model developed by Friedman [13] for permittivity. This notable example that does permit the study of this case, but then only with very special conditions on the microstructural information. Not all applications will possess this; an interesting application is the prediction of the overall properties of resins reinforced with one dimensional carbon nanotubes (fibres) or two dimensional graphene nanoplatelets (discs) [14], due to their light weight and good chemical resistance compared to more conventional materials. In fact, to study the associated properties and based on experimental analysis or well known expressions, analytical models can be employed [15–19]. However, these schemes have a limited applicability, cannot be used for more general geometries and none consider the spatial distribution effect between different phases.

In this work therefore, our aim in this work is to develop the methodology for three-phase HS bounds in order to accommodate geometries and microstructural parameters that incorporate the spatial distribution of the inclusions. It should be noted that the present scheme is certainly not a simple extension of that studied in [20] for the two phase case. Most importantly, the present case describes the interaction, not only between inclusions of the same phase, but also between different phases, to avoid their overlap, thanks to the probability density function introduced in [9]. Therefore, as a consequence, the developed scheme can straightforwardly be employed and extended for the derivation of the HS bounds for multiphase composites. For the particular case of spheroidal inclusions, we analyse the influence of their aspect ratio on the volume fractions of any phase, something that as far as we know has not been clearly described in the literature.

It should be noted that although the general form for the HS bounds applicable to arbitrarily anisotropic composites can be written down in some cases, works concerning the *construction* of such bounds from first principles (volume fractions, elastic or physical properties, shapes of phases of the composite and their spatial distribution) of a given material are not easily found, if they exist at all, particularly for the three phase case.

For all these reasons, using a tensor-basis for transverse isotropy and exploiting the uniformity of the so-called Eshelby and Hill tensors [21], we construct explicit expressions for the HS bounds for the effective quasi-static *transport* properties (thermal or electrical conductivity, electrical resistivity or magnetic permeability) for *transversely isotropic* (TI) *three phase* media, incorporating information as regards the shape, relative size and distribution of the two filler phases.

Using the symmetrical way in which it relates two different types of inclusion phases, the fact that the Mori–Tanaka model cannot be realized from the Ponte Castañeda & Willis method will be graphically exposed. The explicit dependence of the obtained formulae on the microstructural parameters provides the possibility of application to a wide range of geometries and not only the case of spherical inclusions and distributions, which is a frequent assumption.

We illustrate the implementation of the scheme with several examples where comparisons with other theoretical predictions confirm that the present model can predict and bound the effective transport properties with accuracy.

2. Problem statement

It is well known that Laplace's equation governs a significant range of applications, e.g. electrical and thermal conductivity and permittivity, magnetic permeability to name but a few. The mathematical formulation of such problems is therefore identical. In this work to fix notation, we restrict attention to the prediction of the macroscopical electrical conductivity of a

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