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Microstructural efficiency: Structured morphologies

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ABSTRACT

The effective conductivity of binary composites may be estimated through a number of analytical, empirical and numerical methods. These methods must incorporate the relative conductivities, the volume fractions and morphologies of the constituent materials. The concept of microstructural efficiency is introduced in this paper as a means of quantifying the effect of morphology on effective conductivity in a composite. The variation of microstructural efficiency on structured prismatic and three dimensional morphologies is calculated using a Lattice Monte Carlo method. This information enables discussion of the advantages and disadvantages of particular morphologies as conductors or insulators in addition to providing a method for calculating effective conductivity.

1. Introduction

Macroscopic properties of composites allow an engineer or material scientist to make practical decisions on real world applications. A composite may be composed of several constituents which are chemically dissimilar and separated by a distinct interface. How the material properties of the constituents may be homogenised to an effective macroscopic average depends on the particular property. In a thermal study the equilibrium properties of heat capacity and density can be homogenised simply with a mass and volume weighted average respectively. Transient thermal properties like thermal conductivity depend on the morphology of the composite in addition to the constituent properties. Functionally, in a binary composite, that is:

$$\bar{k}_{\text{iso}} = f(k_1, r, \varphi_1, \text{Morphology}) \tag{1}$$

where $\bar{k}_{\text{iso}}$ represents the effective isotropic thermal conductivity of the homogenised composite, k_1 is the isotropic conductivity of the inclusion phase, r is the isotropic conductivity ratio of the two constituents ($r = k_1/k_0$), φ_1 describes the volume fraction of the inclusion phase and the fourth written term refers to the influence of the composite morphology on the effective thermal conductivity. The subscripts 1 and 0 refer to the inclusion and matrix phases respectively. The goal of this paper is to quantify the influence of morphology for structured morphologies.

Though thermal conductivity is taken as the running example in this paper, analogies exist in other physical systems. Table 1 describes some analogues between thermal conductivity and other common engineering situations. These properties are also resolvable with the methodology presented in this paper.

Homogenisation of material properties has been an open field of research for centuries, including contributions from many renowned scientists such as Maxwell and Lord Rayleigh, who made significant contributions through the late 19th century [1,2]. A great number of analytical and empirical methods were developed through the 20th century, before advances in computational resources allowed numerical methods to become widely used. The large body of information available has been summarised through many excellent review articles e.g. [3–6]. The models presented below are far from exhaustive, instead providing well-known work as a point of comparison and example of microstructural efficiency calculation. Modern correlations improve upon these models but rarely is the case of structured morphologies considered [7,8].

The effective conductivity of a composite is known to always fall within the Wiener bounds [6] given by the volume fraction weighted series ($\bar{k}_{\text{ser}}$) and harmonic ($\bar{k}_{\text{har}}$ averages (Eqs. (2) and (3) respectively). The upper limit is the highest effective conductivity possible for a particular composite and is useful for normalisation purposes. There do in fact exist tighter bounds than this as described by Hashin and Shtrikman [9] provided statistical isotropy is attained. However, here we adhere to the upper Wiener bound (Eq. (2)) as the highest possible conductivity.

$$\bar{k}_{\text{ser}} = \varphi_1 k_1 + (1 - \varphi_1) k_0 \tag{2}$$

$$\bar{k}_{\text{har}} = \left(\frac{\varphi_1}{k_1} + \frac{(1 - \varphi_1)}{k_0} \right)^{-1} \tag{3}$$

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The Maxwell–Eucken model (adapted in 1940 by Eucken) is commonly used to estimate the effective conductivity ($\bar{k}_{ME}$) of low concentrations of disperse spheres in a matrix [10]. The model assumes the temperature field about each particle does not interact with those surrounding [11]. Hence it is constrained in validity to volume fractions for which spheres are separated by distance much larger than their diameters.

$$\bar{k}_{ME} = \frac{k_1\varphi_1 + k_0(1-\varphi_1)[3k_1/(2k_1+k_0)]}{\varphi_1 + (1-\varphi_1)[3k_1/(2k_1+k_0)]} \tag{4}$$

The effective mean field theory was first proposed by Bruggeman in 1935 [12] and considers a macroscopically homogeneous distribution of spheres. The validity of mean field theory models break down close to percolation (i.e. long range connectivity) of an inclusion phase. The effective conductivity ($\bar{k}_{Bru}$ in this case is found through implicit solution of the following:

$$1-\varphi_1 = \frac{(k_1-\bar{k}_{Bru})}{(k_1-k_0)}\left(\frac{k_0}{\bar{k}_{Bru}}\right)^{1/3} \tag{5}$$

It should be noted that all four models here do not explicitly depend on the morphology of the medium. Morphological factors may be taken into account using specific semi-empirical and empirical models [5,6,13–15]; however these models often have a small range of validity and require a large number of geometric factors to be specified.

A simple model that considers a specific morphology is the Halpin–Tsai theoretical model [5,15]. It is most appropriate for filaments of uniform cross-sectional area running in parallel through a matrix. The parallel and lateral components of the effective conductivity tensor are separately considered. The parallel component is assumed to be the series volume (or area in this case) weighted average. The transverse components take into account the shape of the filament. The effective isotropic conductivity ($\bar{k}_{HT}$ through this model is:

$$\bar{k}_{HT} = \frac{2}{3}\left(\frac{1+\xi\gamma\varphi_1}{1-\gamma\varphi_1}\right) + \frac{1}{3}(\varphi_1 k_1 + (1-\varphi_1)k_0) \tag{6}$$

Here the additional coefficients are:

$$\gamma = \frac{\frac{k_1}{k_0}-1}{\frac{k_1}{k_0}-\xi}$$

$$\xi = \begin{cases} \sqrt{3}\log\left(\frac{a}{b}\right) \text{ for a plate of width a and height } b \\ 1.0 \text{ for square or circular fibres} \end{cases}$$

Microstructural efficiency was first introduced by Rawson et al. in 2014 [16] as a means of comparing the preferable microstructure for composites of immiscible metals. Here it was found that a Tin–Aluminium composite would be more conductive if it were composed of non-percolating spheres of Tin. It was also found that for a Copper–Iron system, the more highly conductive Copper would benefit from greater percolation. These systems had the additional constraint that the lower melting temperature constituent (Tin and Copper respectively) had to be macroscopically encapsulated so as to form a phase-change thermal storage material [17].

Table 1
Similar transient properties involved in engineering situations.

Situation	Transient property
Temperature field	Thermal conductivity
Electric field	Electrical conductivity
concentration field	Species diffusivity
Electric field applied on a dielectric	Permittivity
Magnetic field	Magnetic permeability

Microstructural efficiency is a convenient property for quantifying the overall impact of morphology on the effective isotropic conductivity of a composite. The microstructural efficiency (η_μ) is defined as the ratio of the actual (measured or computed) effective isotropic conductivity ($\bar{k}_{iso}$) to the volume weighted series average of the constituents. If φ_i is the volume fraction of the ith constituent the functional form may be written:

$$\eta_\mu = \frac{\bar{k}_{iso}}{\sum_{i=1}^{n}\varphi_i k_i} \tag{7}$$

If the microstructural efficiency were available for a given morphology then the effective isotropic conductivity could be easily back calculated, from:

$$\bar{k}_{iso} = \eta_\mu\ \bar{k}_{ser} \tag{8}$$

This paper documents the microstructural efficiency of binary composites for seven different structured morphologies over a range of volume fractions and conductivity ratios. Structured morphologies remove the degree of freedom brought around by random packing and often have clearly defined percolation volume fractions. Considering these well studied morphologies facilitates discussion on more general random morphologies in future work.

To produce microstructural efficiency data the effective isotropic conductivity for the particular morphology, volume fraction and conductivity ratio must be found. The effective isotropic conductivity may be obtained through a number of means. The analytical and empirical methods discussed earlier may be used although these are limited to certain morphologies. For completely general morphologies, numerical methods can provide a much more flexible approach.

The Lattice Monte Carlo (LMC) numerical method has been successfully utilised in the determination of effective isotropic conductivity for a number of morphologies [16,18–21]. The LMC method involves simulating heat diffusion at steady state through random walks of particles over a lattice. The lattice describes the location and relative conductivity of the constituents giving a representation of the composite morphology. A repeating volume of the lattice is simulated with the introduction of periodic boundaries. The effective diffusivity is inferred by the Einstein diffusion equation. The effective diffusivity with unity thermal inertia (simulated at steady state) is by definition the effective thermal conductivity [22], thus the following holds:

$$\bar{k}_{iso} = \frac{\langle R^2\rangle}{2dt} \tag{9}$$

Here R refers to the displacement of a particle, d is a constant related to the dimensionality of the simulation and t is the number of time steps.

As the LMC method must discretise a domain to a (usually cubic) grid, the number of nodes employed must be high enough such that the morphology is adequately represented. This validation step is common in discrete and finite element analyses and is often referred to as the establishment of mesh independence. It was found by Rawson et al. that a sphere discretised with more than ten nodes across its radius in a random hard sphere morphology would achieve mesh independence in effective isotropic thermal conductivity [16]. Additionally where the inclusions have a very small separation or intersection, the grid must be fine enough to resolve the fine feature. This can be ensured by calculating the separation or intersection and ensuring the lattice spacing is smaller.

The LMC method has an inherent statistical uncertainty which is approximately inversely proportional to the square root of the number of particles simulated. This uncertainty can be reduced below an acceptable proportion by simply increasing the particle