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n-Phase micromechanical framework for the conductivity and elastic modulus of particulate composites: Design to microencapsulated phase change materials (MPCMs)-cementitious composites

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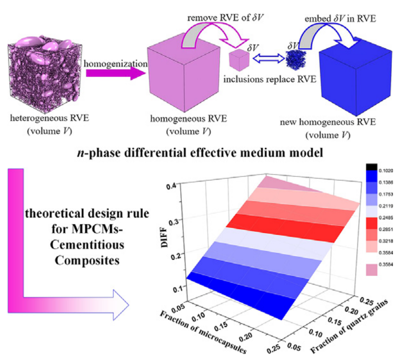
HIGHLIGHTS

- *n*-phase differential model for effective properties is devised with a good accuracy.
- The *n*-phase model suits composites with multiple inclusions and interfaces.
- The advanced performance of MPCM-CC is smartly designed for the first time.
- The results can apply to the composite design of other particulate materials.

GRAPHICAL ABSTRACT



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ABSTRACT

The smart design of microencapsulated phase change materials (MPCMs) in cementitious composites requires an explicit understanding of effects of soft microcapsule particles, stiff aggregates and their surrounding weak interfaces on the physico-mechanical properties of particulate composites. This paper devises a *n*-phase micromechanical framework to predict the effective thermal conductivity and elastic modulus of multicomponent particulate composites that consist in stiff and soft anisotropic-shaped inclusions, their surrounding weak interfaces and matrix. In this micromechanical model, the volume fraction of weak interfaces treated as the interphase model is quantified and incorporated into the *n*-phase differential effective medium model. It is found that the structural configuration of interfaces has a significant effect on the effective physico-mechanical properties of particulate composites. The micromechanical model leads to predictions of the effective conductivity and elastic modulus of multicomponent particulate composites to a good accuracy by comparing with available experimental data for regular concrete, quartz mortar and MPCMs-cementitious composites. By utilizing the micromechanical model, the authors further develop a theoretical design rule for the robust overall performance of MPCMs-cementitious composites with the better thermal resistance and elastic modulus. These results can also be used to design other multiphase particulate composites and porous media with the cherry-pit structure.

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1. Introduction

Microencapsulated phase change materials (MPCMs) have attracted increasingly attention of materials research community due to their economic feasibility to the enhancement of thermal energy storage in cementitious composites. It is well known that the embedment of microcapsules encapsulated by phase change materials (PCM) in cementitious composites is an effective means to create smart building materials suitable for green passive house construction [1,2]. However, recent experimental explorations found that the addition of PCM-microcapsules degrades the mechanical properties (e.g., elastic modulus and compressive strength) of cementitious composites [2–5], contributing to the elastic modulus and strength of microcapsules as soft inclusions far inferior to the binder matrix [3–5] and the weak interfacial effect between microcapsules and matrix [2]. The smart design of a robust MPCMs-cementitious composite (MPCMs-CC) requires an explicit understanding of the interplay among components, structures and physico-mechanical properties like thermal conductivity and elastic modulus. Unfortunately, the three quantitative relationships are difficultly elucidated through expensive or time-consuming laboratory explorations because of the complexity of interplay of component-structure-property. Therefore, for reasons of material design, it is necessary to develop a powerful predictive toolkit to explicitly understand the interplay of component-structure-property in MPCMs-CCs.

In recent years, some efforts have been devoted to theoretically and numerically predicting the effective thermal conductivity and elastic modulus of MPCMs-CCs. For instance, Meshgin and Xi [6] attempted different composite models like the bounds model, Maxwell model and generalized self-consistent scheme to evaluate the effective thermal conductivity of MPCMs-concrete. Sant and co-workers [7,8] utilized the finite element method to calculate the thermal conductivity and elastic moduli of three-phase MPCMs-CCs composed of matrix and microcapsule particles considering spherical core-shell structure. Other numerical schemes have also been presented to investigated mechanical properties of multiphase concrete-like particulate composites [9–12]. A comprehensive review on components, microstructures and physico-mechanical properties of numerical concrete has been summarized by Xu and coworkers [13,14]. Although these predominant contributions may provide guidance for the effective physico-mechanical properties of MPCMs-CCs, the assumption of isotropic spherical particles cannot reflect the anisotropy nature of inclusions like aggregates in MPCMs-CCs. Plus, the interfacial effect around microcapsule particles has received relatively little attention until fairly recently [2]. Cui et al. [2] observed that the weak bond between MPCMs and the binder matrix can induce the interfacial gap between MPCMs and mortar through experiments. Actually, there have been numerous homogeneous models formulated to predict the effective physico-mechanical properties of three-phase composites considering anisotropic inclusions and interfaces, such as the effective medium approximations [15–17], the generalized self-consistent method [18,19], Mori-Tanaka model [20], double-/multiple-inclusion models [21,22], differential effective medium (DEM) approximations [23,24] and other effective medium methods [25,26]. Xu et al. [13,14] have recently summarized the existing theoretical studies in this field. These models are helpful to understand the effects of stiff anisotropic inclusions and weak/reinforced interfaces on the physico-mechanical properties of composites. Nevertheless, very far few theoretical works have probed the physico-mechanical properties of multiphase composites (more than three phases) containing anisotropic hard/soft inclusions and weak interfaces. MPCMs-cementitious composite is essentially a multiphase and multiscale particulate composite that is composed of matrix, stiffer aggregates of irregular shapes, softer microcapsule particles and their surrounding weak interfaces with different physical configurations. The estimation of conductive and elastic properties of such multiphase composite materials remains open so far. It is our intention in the present work to address this gap.

This paper attempts to develop a n-phase micromechanical framework for understanding the effects of the combination of anisotropic stiff grains and soft microcapsule particles and their surrounding interfaces on the effective conductivity and elastic modulus of multiphase particulate composites. In this framework, inclusion shapes cover spherical, ellipsoidal, cylindrical and disc shapes. The conductivity and elastic modulus of each constituent as well as their volume fractions, especially the weak interfacial volume fraction, are taken into consideration. The predicted effective conductivity and elastic modulus from the present model are compared with available experimental data. Furthermore, applying the micromechanical framework, we propose a design rule for MPCMs-CCs with the better thermal resistance and elastic modulus. The results of this study could also be applicable to other multicomponent composites like self-healing microcapsule-embedded cementitious composites, lightweight concrete and self-healing polymer composites, to name but a few.

2. *n*-Phase micromechanical framework

2.1. Two-phase DEM model

The differential effective medium (DEM) theory stemmed from Bruggeman [27], has been broadly applied to evaluate the effective elastic, conductive and diffusive properties of two-/three-phase composites [23,24,28–32]. It consists in building up a composite material through a process of incremental homogenization. As pointed out by Hashin and Shtrikman [33], the theoretical predictions of these effective parameters like the thermal/electrical conductivity, permeability, elastic modulus and diffusivity of heterogeneous composites are mathematically analogous. Also, these effective parameters may transform each other through the classical Nernst-Einstein relationship [34,35]. Considering a representative volume element (RVE) of heterogeneous two-phase composites consists in homogeneous matrix as phase 1 with its physico-mechanical property ε_1 (representing the diffusivity, conductivity or elastic modulus) and the volume fraction ϕ_1, and inclusions as phase 2 with its physico-mechanical property ε_2 and the volume fraction ϕ_2. These inclusions are randomly distributed in matrix like cement paste, which can be viewed as a statistically homogeneous RVE. The DEM incremental homogenization for the two-phase model can be schematically displayed in Fig. 1, and its mathematical derivation is explicitly formulated in Supplementary Information (see S1). In this text, we directly give the explicit expressions on the effective physico-mechanical property ε of two-phase composites with inclusions of various geometric shapes like spherical (Eq. (1)), ellipsoidal (Eq. (2)), cylindrical (Eq. (4)) and disk (Eq. (5)).

$$1-\phi_2=\left(\frac{\varepsilon_1}{\varepsilon}\right)^{\frac{1}{3}}\left(\frac{\varepsilon-\varepsilon_2}{\varepsilon_1-\varepsilon_2}\right),\text{ spherical} \tag{1}$$

It can be seen that Eq. (1) is in good line with those for the effective diffusivity and elastic modulus of concrete with spherical aggregates reported by Garboczi et al. [29], and those of the effective elastic modulus of rocks with spherical pores displayed by Markov et al. [32].

$$1-\phi_2=\left(\frac{\varepsilon_1}{\varepsilon}\right)^{A}\left(\frac{\varepsilon-\varepsilon_2}{\varepsilon_1-\varepsilon_2}\right)\left(\frac{\varepsilon_1+B\varepsilon_2}{\varepsilon+B\varepsilon_2}\right)^{C},\text{ ellipsoidal} \tag{2}$$

where $A = 3L_1(1-2L_1)/(2-3L_1)$, $B = (2-3L_1)/(1+3L_1)$, and $C = -2(3L_1-1)^2/(9L_1^2-3L_1-2)$. L_1 is the depolarization factor of spheroidal inclusions that is given by [19,21].

$$L_1=\begin{cases}\frac{1}{2}\left\{1+\frac{1}{\kappa^2-1}\left[1-\frac{\kappa}{2\sqrt{\kappa^2-1}}\ \ln\left(\frac{\kappa+\sqrt{\kappa^2-1}}{\kappa-\sqrt{\kappa^2-1}}\right)\right]\right\}, & \kappa>1\\ \frac{1}{2}\left\{1+\frac{1}{\kappa^2-1}\left[1-\frac{\kappa}{\sqrt{1-\kappa^2}}\ \tan^{-1}\left(\frac{\sqrt{1-\kappa^2}}{\kappa}\right)\right]\right\}, & \kappa<1\end{cases} \tag{3}$$