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Effective elastic moduli of core-shell-matrix composites

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ABSTRACT

The effective Young's modulus and Poisson's ratio of spherical monodisperse and polydisperse core-shell particles ordered or randomly distributed in a continuous matrix were predicted using detailed three-dimensional numerical simulations of elastic deformation. The effective elastic moduli of body-centered cubic (BCC) and face-centered cubic (FCC) packing arrangements of monodisperse microcapsules and those of randomly distributed monodisperse or polydisperse microcapsules were identical. The numerical results were also compared with predictions of various effective medium approximations (EMAs) proposed in the literature. The upper bound of the EMA developed by Qiu and Weng (1991) was in good agreement with the numerically predicted effective Young's modulus for BCC and FCC packings and for randomly distributed microcapsules. The EMA developed by Hobbs (1971) could also be used to estimate the effective Young's modulus when the shell Young's modulus was similar to that of the matrix. The EMA developed by Garboczi and Berryman (2001) could predict the effective Poisson's ratio, as well as the effective Young's modulus when the Young's modulus of the core was smaller than that of the matrix. These results can find applications in the design of self-healing polymers, composite concrete, and building materials with microencapsulated phase change materials, for example.

1. Introduction

PCMs are thermal energy storage materials that can store a large amount of energy in the form of latent heat (Ling and Poon, 2013). Substantial interest exists in embedding phase change materials (PCMs) into building materials, such as mortars, concrete, and gypsum wallboard, in order to improve building energy efficiency (Ling and Poon, 2013; Tyagi and Buddhi, 2007; Farid et al., 2004; Sharma et al., 2009; Tyagi et al., 2011; Salunkhe and Shembekar, 2012; Khudhair and Farid, 2004; Cabeza et al., 2007; Hunger et al., 2009). In such applications, organic PCMs are encapsulated in microcapsules with a median diameter between 1 μm and 1 mm, and a capsule thickness of a few microns, to prevent (i) the leakage of liquid PCM, (ii) reaction with the cementitious matrix, and (iii) to minimize the risk of flammable organic PCMs (Farid et al., 2004; Sharma et al., 2009; Tyagi et al., 2011; Salunkhe and Shembekar, 2012; Fernandes et al., 2014). Typically, the encapsulation (e.g., melamine-formate), and the encapsulated PCM (e.g., a paraffin) demonstrate

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mechanical properties (e.g., elastic modulus, strength) far inferior to the cementitious matrix. As a result, the inclusion of PCM microcapsules into cementitious systems results in degradation of mechanical properties, in proportion to the inclusion volume (Hunger et al., 2009; Fernandes et al., 2014). Thus, for reasons of structural (building) design, it is necessary to understand how the inclusion of PCMs influences the mechanical properties of cementitious composites. Similarly, in composite concrete, chemical reactions between aggregates and the cement paste result in the development of the so-called interfacial transition zone (ITZ) between the two materials (Mindess et al., 2003). This type of concrete could also be modeled as a three-component core-shell-matrix composite, with the aggregates, ITZ, and cement paste corresponding to the core, shell, and matrix components, respectively.

Other applications of three component core-shell-matrix composites include self-healing polymer composites (Brown et al., 2004; White et al., 2001). This composite material consists of microcapsules filled with healing agents such as dicyclopentadiene (DCPD) embedded in an epoxy matrix. When the polymeric capsules are ruptured by a propagating crack, the encapsulated healing agent is released, thus sealing the crack (Brown et al., 2004). Such self-healing polymers have applications in the aviation industry, where cracking is a major safety hazard (Ghosh, 2009).

In all the aforementioned applications, predicting the material's mechanical response to various loading conditions is essential to the material selection and design. There exists a wide range of micromechanical models formulated to predict the effective elastic properties of multicomponent composites. The vast majority of these models account for the presence of an inclusion stiffer than the surrounding matrix, rather than softer. In addition, they were often derived by considering a single microcapsule in an infinitely large matrix. Finally, there exist so many different effective medium approximations that one wonders which one is the most appropriate. The present study aims to rigorously predict the effective elastic moduli of three-component core-shell-matrix composites through numerical simulations of a wide range of microcapsule size and spatial distributions as well as volume fractions and mechanical properties of the constituent materials.

Nomenclature

$\mathbf{C}$	stiffness tensor, GPa
D	diameter, μm
E	Young's modulus, GPa
G	shear modulus, GPa
$\mathbf{I}$	fourth-order identity tensor
K	bulk modulus, GPa
L	unit cell length, μm
N	number of unit cells
$\mathbf{S}$	Eshelby tensor
$\mathbf{u}$	displacement vector, m
u	displacement in the x-direction, m
v	displacement in the y-direction, m
w	displacement in the z-direction, m
Symbols	
ϕ	volume fraction
ν	Poisson's ratio
λ	Lamé's first parameter, GPa
μ	Lamé's second parameter, GPa
σ	normal stress, MPa
τ	shear stress, MPa
$\boldsymbol{\sigma}$	Cauchy stress tensor, MPa
$\boldsymbol{\epsilon}$	infinitesimal strain tensor
ϵ	normal strain
γ	shear strain
Subscripts	
c	refers to core
eff	refers to effective properties
m	refers to matrix
s	refers to shell
$c+s$	refers to core-shell particle

2. Background

2.1. Mechanical properties of materials

Linear elastic constitutive relationships for an isotropic material are given by Hjelmstad (2005)

$$\boldsymbol{\sigma} = \mathbf{C} : \boldsymbol{\epsilon} \tag{1}$$

where $\boldsymbol{\sigma}$ and $\boldsymbol{\epsilon}$ are the stress and strain tensors, respectively, and $\mathbf{C}$ is the fourth-order stiffness tensor. The latter is a property of the material and depends on its microstructure and temperature. The same expression can be written in component form as,

$$\sigma_{ij} = C_{ijkl}\,\epsilon_{kl} \tag{2}$$

where summation is implied over repeated indices, and their ranges are given as $\{i, j, k, l\} \in \{1, 2, 3\}$. For homogeneous and isotropic materials, the tensor $\mathbf{C}$ is given by

$$C_{ijkl} = \lambda\delta_{ij}\,\delta_{kl} + \mu(\delta_{ik}\,\delta_{jl} + \delta_{il}\,\delta_{jk}) \tag{3}$$

where λ and μ are the Lamé parameters, and $\delta_{\alpha\beta}$ denotes a Kronecker delta. The material tensor in Eq. (3) can also be expressed in terms of other well known elastic moduli, using the following identities

$$\lambda = \frac{E\,\nu}{(1+\nu)(1-2\nu)} = K - \frac{2}{3}G, \quad \mu = \frac{E}{2(1+\nu)} = G \tag{4}$$

where E, K, and G are, respectively, the Young's, bulk, and shear moduli, while ν is the Poisson's ratio.

2.2. Effective medium approximations

Effective medium approximations (EMAs) have been formulated to predict the effective elastic moduli of three-component core-shell-matrix composites. Various expressions of EMAs developed for $E_{\rm eff}$, $\nu_{\rm eff}$, $G_{\rm eff}$, and $K_{\rm eff}$ as functions of the elastic moduli of the core (subscript c), the shell (subscript s), and the matrix (subscript m) and of their respective volume fractions, denoted by ϕ_c, ϕ_s, and ϕ_m, are discussed in the next section. Some EMAs use the core-shell volume fraction defined as $\phi_{c+s} = \phi_c + \phi_s$ (Qiu and Weng, 1991; Herve and Zaoui, 1993).