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Strategy for interfacial overlapping degree in multiphase materials with complex convex particles

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ABSTRACT

Determining the overlapping degree of interfaces around solids is an open problem with great significance in a variety of materials. So far, this search has been performed only on a case-by-case basis, particularly for hard spherical particles. Here, we present a generalized scheme to evaluate analytically the interfacial overlapping degree with complex convex particles. It is essentially an extension of spheres to complex convex particles like convex polyhedrons and ellipsoids for the interfacial overlapping degree. Additionally, a numerical model is also proposed to numerically derive the interfacial overlapping degree on the basis of the Minkowsky addition manner. Comparing with the theoretical data reported in the literature and numerical results from the present numerical model, the proposed theoretical scheme is confirmed with a favorable reliability. Furthermore, we find a quantitative mechanism between the interfacial overlapping degree and the surface configurations of convex particles. Such a mechanism can be used as a theoretical criterion to provide guidance for practical industries of composite media.

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1. Introduction

Understanding microstructures of interfaces, such as the interfacial thickness, volume fraction, and percolation, is a central challenge in materials with discrete solid particles of irregular geometries [1–3]. It is in fact that geometric configurations of discrete particles play an essential role in assessing the microstructures of interfaces. Experimental studies have confirmed that interfaces around particles are a complex network structure, since adjacent interfaces can have a high overlapping degree [4,5]. Despite the importance of the overlapping degree of interfaces in the prediction of mechanical and transport behaviors of multiphase materials like colloids [6], granular composites [7], ceramics, and concrete [8], it is a difficult task to capture such information on the interfacial overlapping degree by experimental investigations.

As an interesting parameter, the interfacial overlapping degree characterizes the state of overlap of interfaces in multiphase materials. Theoretical and numerical efforts have been made to obtain the overlapping degree of interfaces around solid particles. One approach is to consider multiphase materials as a three-phase composite cell consisting of polydisperse solid particles, soft interfaces with a constant thickness attached onto the surface of each particle, and matrix, this is also known as the hard core/soft shell structure [9]. By virtue of the hard core/soft shell structure, researchers investigated the volume fraction of interfaces around spherical particles [10,11], of which the derivation was actually dependent on the theory of the nearest-surface distribution functions developed by Lu *et al.* [12]. Accordingly, Xu *et al.* [13] further put forward to the interfacial overlapping degree around spheroidal particles as an expression of the volume fraction of interfaces, that is,

$$IOD = \frac{V_{hi} - V_{si}}{V_{si}} \quad (1)$$

where IOD is the interfacial overlapping degree, V_{si} is the volume fraction of soft interfaces, and V_{hi} is the volume fraction of hard interfaces that is defined as the interfacial layers without any overlap in the three-phase composite structure. Also, the results revealed that the overlapping degree is dependent on the aspect ratio of spheroidal particles [13]. Although the preponderance of these previous works is of importance for understanding the effect of the particle geometry on the interfacial overlapping degree, more complex convex particles that may contain specific corner angles and facets should be focused, since solids are normally not perfect spheres or ellipsoids in multiphase materials as discussed in the literature. Virtually, recent studies have

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claimed that the microstructural characteristics of interfaces are controlled by the surface configuration of solid particles, through evaluating the thickness and volume fraction of interfaces around ellipsoidal and polyhedral particles [14]. However, it remains dubious how the interfacial overlapping degree is dependent on the surface configurations of complex convex particles. It is our objective in this work to address this gap.

This article attempts to develop a theoretical model to bridge the gap between the interfacial overlapping degree and the surface configurations of complex convex particles. The remainder of this article is organized as follows: In Section 2, the generalized theoretical scheme for the interfacial overlapping degree with convex particles is established. Subsequently, the proposed scheme is tested and discussed in Section 3. The final section displays our conclusions.

2. Theoretical scheme

As a theoretical foundation of the interfacial overlapping degree, the theory of the nearest-surface distribution functions will be reviewed briefly to formulate the theoretical scheme with convex particles. The theory of the nearest-surface distribution functions was firstly put forward by Lu and Torquato [12], in which a so-called spherical void exclusion probability representing in fact the volume fraction of a matrix in a two-/three-phase composite structure was derived by applying the statistical geometry of composites and the theory of geometrical probability. Afterwards, it has been extensively applied to compute the volume fraction of soft interfaces in a composite cell mentioned above [10,12–16]. For instance, in a three-phase composite structure composed of a matrix, convex particles and soft interfaces with a constant thickness, as shown in Fig.1, the volume fraction of the matrix can be denoted as [3,14]

$$V_m = (1 - V_p)\exp\left[-\pi N_V\left(et + dt^2 + gt^3\right)\right] \quad (2)$$

where V_m and V_p are volume fractions of the matrix and solid particles, respectively. t is the interfacial thickness, N_V is the number density of solid particles in the three-phase composite structure, the parameters e, d, and g are dependent on the geometric configurations of hard particles. For convex particles, the parameters e, d, and g are expressed as [3,13,14]

$$e = \frac{S_V}{\pi N_V (1 - V_p)} \quad (3)$$

$$d = \frac{2\langle D_{eq}\rangle}{1 - V_p} + \frac{S_V^2}{2\pi N_V (1 - V_p)^2} \quad (4)$$

$$g = \frac{4}{3(1 - V_p)} + \frac{2S_V\langle D_{eq}\rangle}{3(1 - V_p)^2} + \frac{mS_V^3}{27\pi N_V (1 - V_p)^3} \quad (5)$$

where S_V is the specific surface area of solid particles. The parameter m depends on a theoretical approximation of the radial distribution function, such as $m = 0$ being the Percus–Yevick approximation [17], $m = 2$ being the Carnahan–Starling approximation [18], $m = 3$ being the scaled-particle approximation [19]. The kth moment $\langle D_{eq}^k\rangle$ of area of f_N (D_{eq}) about the origin is displayed by

$$\left\langle D_{eq}^k\right\rangle = \int_{D_{\min eq}}^{D_{\max eq}} D_{eq}^k f_N(D_{eq})\,\mathrm{d}D_{eq} \quad (6)$$

where f_N (D_{eq}) is the number-based probability function representing the particle size distribution. $D_{\max eq}$ and $D_{\min eq}$ are the maximum and minimum equivalent diameters of convex particles, respectively. According to the quantitative stereology [20], S_V for convex particles can be written as

$$S_V = \frac{6V_p\left\langle D_{eq}^2\right\rangle}{s\left\langle D_{eq}^3\right\rangle} \quad (7)$$

where s is a sphericity defined as the ratio between the surface area of a sphere and that of a solid particle with the same volume [21,22]. In this work, each particle in a system is predefined to possess the same sphericity to assess the effect of the surface configuration of convex particles. Thus, on the basis of the theory of composites, the volume fraction of soft interfaces around convex particles can be given by

$$V_{si} = 1 - V_p - V_m = (1 - V_p)\left\{1 - \exp\left[-\pi N_V\left(et + dt^2 + gt^3\right)\right]\right\} \quad (8)$$

According the definition of the interfacial overlapping degree described above, the volume fraction of hard interfaces of which are without any overlap needs to be derived for formulating the interfacial overlapping degree. Supposed that an arbitrary convex particle $\mathbf{C}_1$ with the equivalent diameter D_{eq1}, an interface with a constant thickness t around $\mathbf{C}_1$ can be realized by the Minkowsky addition manner [23,24], that is,

$$A \oplus B = \{\mathbf{X} + \mathbf{Y} | \mathbf{X} \in A, \mathbf{Y} \in B\} \quad (9)$$

where A and B denote two geometric sets. $\mathbf{X}$ and $\mathbf{Y}$ are point vectors representing geometric profiles of A and B, respectively. The above relationship equals geometrically to the profile derived by sweeping one set around the other, without changing their relative position and orientation. In Fig. 2, for instance, the real geometric morphology of the interfacial shell with a constant thickness around a tetrahedron is performed by the Minkowsky sum of the tetrahedron with a sphere with the radius equivalent to the interfacial thickness and its center located on the surface of the tetrahedron.

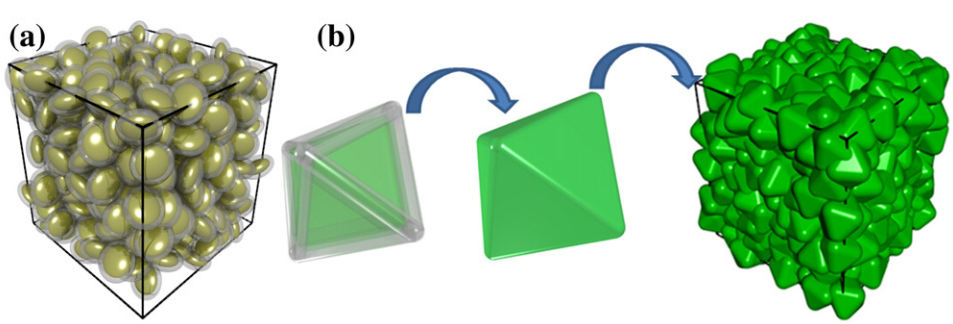

Fig. 1. Schematic views of the three-phase composite cells composed of (a) ellipsoidal particles, soft interfaces and matrix, (b) convex octahedral particles, soft interfaces and matrix. (a) In the ellipsoidal particle system, yellow ellipsoids represent hard solids and the external transparent shell around each yellow ellipsoid stands for its interfacial layer, the remainder region is just matrix. Similarly, (b) in the convex octahedral particle system, green octahedrons represent hard solids and the external transparent shell around each green octahedron characterizes its interfacial layer.

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