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Percolation phase diagrams for multi-phase models built on the overlapping sphere model

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HIGHLIGHTS

- New, multi-phase model built on the classic overlapping sphere model.
- Percolation thresholds up to 50% less than overlapping sphere threshold.
- Explicit percolation phase diagrams for up to 4 phases, implicitly for N phases.

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ABSTRACT

The overlapping sphere (OS) percolation model gives a two-phase microstructure (matrix plus inclusions) that is useful for testing composite material ideas and other applications, as well as serving as a paradigm of overlapping object percolation and phase transitions. Real materials often have more than two phases, so it is of interest to extend the applicability of the OS model. A flexible variant of the OS model can be constructed by randomly assigning the spheres different phase labels, according to a uniform probability distribution, as they are inserted one by one into the matrix. The resulting three or more phase models can have different amounts of percolating and non-percolating phases, depending on the volume fraction of each phase and the total OS volume fraction. A three-dimensional digital image approach is used to approximately map out the percolation phase diagram of such models, explicitly up to four phases (one matrix plus three spherical inclusion phases) and implicitly for $N > 4$ phases. For the three phase model, it was found that a single OS sub-phase has a percolation threshold that ranges from about a volume fraction of 0.16, when the matrix volume fraction is about 0.01, to about 0.30, at a matrix volume fraction of about 0.7. The approximate analytical dependence of this sub-phase percolation threshold on the defining model parameters serves to guide the building of the percolation phase diagram for the N-phase model, and is used to determine the maximum value of N ($N = 6$) at which all N phases can be simultaneously percolated.

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1. Introduction

The percolation aspects of the overlapping sphere model and models based on other overlapping objects have been extensively studied [1–6]. This model gives a two-phase microstructure (matrix plus inclusions) that is useful for testing out composite material ideas and other applications [1], as well as serving as a paradigm of overlapping object percolation and phase transitions. However, real materials often have more than two phases, some of which are percolated (i.e. connected in all directions) and some of which are not (i.e. consisting of isolated clusters). It would be useful to be able to readily construct

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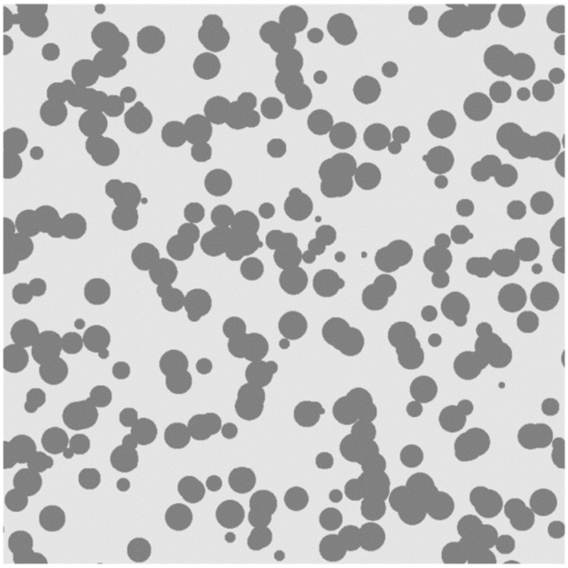

Fig. 1. Slice of the two-phase overlapping spheres (2POS) model. Phase 1 is light gray, and phase 2 is dark gray. 41 voxel diameter spheres in 800^3 voxel unit cell.

model composites in which the continuity of the phases could be controlled for more than two phases. When more than one phase is simultaneously percolated, such a model has been called an interpenetrating phase composite [7].

A simple but flexible variant of the overlapping sphere model can be constructed by randomly assigning the spheres different phase labels, according to a uniform probability distribution, as they are inserted one by one into the matrix. The resulting three or more phase models can have different numbers of percolating and non-percolating phases, depending on the volume fractions of each phase and the overall volume fraction of inserted spheres. A three-dimensional (3D) digital image approach, similar to that used previously in two-dimensional (2D) models [8], is useful for this kind of spatially complicated model and can be employed to approximately map out the percolation phase diagram of such models. A 3D digital image approach, albeit a more sophisticated one, has been used for the matrix percolation problem in similar overlapping object models [9,10]. In this paper, no physical length scale is assigned to the voxels so as to maximize the flexibility of the model, though of course for any comparison to experiment a length scale must be selected. The best known determination of the percolation threshold for the two phase overlapping sphere model [11] and the percolation of the matrix surrounding the spheres [12–15] is used to guide the construction of the phase diagram and help determine the errors caused by using a digital image model.

2. Model description and digital image approach

The classic two-phase overlapping sphere (2POS) model consists of inserting monosize spheres randomly into a matrix, allowing them to freely overlap. The order of placement of the spheres does not matter, since they are all identical. In a two phase infinite system of matrix (phase 1) plus identical, randomly centered and oriented overlapping objects (phase 2), which actually can be of any shape, the volume fractions are given by [3,16,17]:

$$\varphi_1 = \exp(-nV_o) \qquad \varphi_2 = 1 - \exp(-nV_o) \tag{1}$$

where V_o equals the volume of one object and $n =$ the number of objects per unit volume. For any finite realization of this kind of microstructure, even if continuum rather than digital objects are used, Eq. (1) will be an estimate only. A single slice of the 2POS model is shown in Fig. 1 using 41 voxel diameter overlapping spheres, centered on a voxel center, in an 800^3 voxel unit cell, with periodic boundary conditions. The approximate factor of 20 between the sphere diameter and the unit cell size will make any finite size effects negligibly small, as will be seen below. In the system shown in Fig. 1, 5738 spheres were placed and $V_o = 36\,137$ voxels. Eq. (1) then predicts a value of 0.6670 for the matrix volume fraction, a value very close to the actual matrix phase fraction of 0.6656. The small difference is mostly due to the fact that these are digital spheres, and are centered on simple cubic lattice points, not at any point in the unit cell. A burning algorithm was used to determine that both phases were percolated [1]. The sphere phase was expected to be percolated since its volume fraction, 0.3344, was greater than 0.2895 ± 0.0005, the percolation threshold for the sphere phase determined for the 2POS model [11]. The matrix phase in the 2POS model only becomes disconnected at a volume fraction below about 0.03 [12–15].

Based on the above results for the 2POS model, for ϕ_1 between about 0.03 and 0.71, both phases are percolated, while for ϕ_1 greater than 0.71, only phase 1 is percolated, and for ϕ_1 less than 0.03, only phase 2 is percolated. This, in words, is the one-dimensional (1D) percolation phase diagram for the 2POS model, where the only parameter is ϕ_1.