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Determining the representative volume element size for three-dimensional microstructural material characterization. Part 1: Predictive models

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HIGHLIGHTS

- Representative volume elements (RVE) are frequently used for analysis of 3D materials.
- An approach is developed to estimate RVE size for property measurements.
- Volume fraction, particle size, and network contiguity properties are considered.
- Statistical and numerical approaches are developed in the context of simplified structures.
- Results presented graphically to help guide future research.

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ABSTRACT

Recent advances in microstructural imaging and characterization tools have led to an increase in the direct examination of 3-D microstructures of composite materials in devices such as solid oxide fuel cells, battery electrodes, and composite gas separation membranes. In particular, focused ion beam-scanning electron microscopy and x-ray nanotomography methods have opened the door for materials characterization at the tens of nanometer scale. These experimental methods have enabled the quantitative evaluation of microstructures for a variety of important parameters. However, there is often uncertainty in the literature regarding the necessary size of a representative volume element (RVE) in order to capture an accurate description of the structure. In an effort to provide guidance for the field, in this work simplified geometric models are presented to provide basis for the *a priori* estimation of RVE size for three common microstructural parameters: volume fraction, particle size, and network contiguity. In a second and complementary paper (Part 2), the results of the model will be compared to experimental data obtained from the extensive imaging of a multiphase composite membrane material using x-ray nanotomography.

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1. Introduction to the RVE concept

In the study of material microstructures, the characterization of a large material domain can often be simplified by considering a smaller sub-section of the material termed a representative volume element (RVE). The RVE is used to link the heterogeneities at the microscale with effective parameters used to describe the material at the macroscale. The motivation to study materials via an RVE is that it permits smaller computational and experimental domains while still maintaining a description of material behavior relevant to device performance. The RVE concept has been used extensively in the field of continuum mechanics to describe the stress and strain fields within composite materials [1–7]. These studies are typically concerned with predicting the effective physical properties of the material under mechanical load, namely the elastic modulus. However, with recent developments in high resolution 3-D imaging capabilities, the RVE concept has been extensively applied in terms of accurate characterization, as well as simulation, of morphological properties in real physical systems. In particular,

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focused ion beam-scanning electron microscopy (FIB-SEM) and x-ray nanotomography methods capable of resolving the detailed distribution of multiple solid phases at the nanometer scale have helped move towards bridging the gap of understanding the connections between microscale material features and macroscale device performance [8–12].

Several researchers have explicitly considered the effect of the imaging volume size on characterization results [13–21]. From a characterization perspective, the goal of the experimentalist is to sample just a small portion of a total material domain, and in considering just this small region, be able to generate a description that will represent the whole material. For this to be possible, an RVE extracted from any location within the material must statistically contain approximately the same structure and properties as any other randomly selected RVE. This requires the RVE to include a sufficient sampling of the variety of microstructural features that exist in the sample, such that a smaller sub-volume will contain an inadequate sampling of these features and therefore not be representative, while a larger sub-volume will contain more than a sufficient number of features and therefore will also be statistically representative. In that light, we seek a minimum RVE size, understanding that larger sub-volumes can also be used as an RVE. Implicit in this definition is the assumption that the bulk material displays a level of statistical homogeneity at some length scale. In other words, on a local scale the material may have a variety of heterogeneous structures, phases, and complex geometries that are arranged in a specific way unique to that exact location, but on a statistical basis the effective properties of the multiphase material are uniform across a much larger length scale. This would, for example, exclude graded structures in which a property such as particle size or volume fraction has been intentionally varied across the structure during the fabrication process.

In this study, for the sake of uniformity and general applicability, sub-volumes extracted from a total material domain will be restricted to cubic geometries. This is done to remove some of the ambiguity involved in defining RVE sizes based purely on volume, in which case it is not clear over what range of geometry (aspect ratio and shape) that definition is applicable. It is realized that the measurement of some properties depends solely on a count of some feature, such as the number of particles (and therefore volume fraction) of a given phase. For these types of “counting” property measurements, only the total volume that is analyzed, and not the volume's geometry, is significant. However, for some property measurements, particularly those aimed at describing pathway-dependent transport, the characterization results will almost certainly not be the same for two RVE's with very different aspect ratios even if the total volume is the same due to the influence of the boundaries. Therefore, the cube has been chosen here as the standard shape, realizing that that restriction could be relaxed in some instances if desired.

The challenge to the experimentalist is that when imaging is to be performed on a given sample, the minimum RVE size to obtain accurate characterization results is generally not known *a priori*. Furthermore, the necessary size of an RVE may vary depending on the material property and level of precision in which the researcher is interested. In the literature, typically 3-D image data is therefore analyzed after imaging to assess if volume-independent conditions have been met. In an effort to contribute to some predictive capabilities, this work outlines simplified models aimed at estimating the minimum RVE size for several common microstructural properties: volume fraction, phase size distribution, and network contiguity. In Part 2 of this work, the models are compared to experimental results obtained through extensive x-ray nanotomography imaging of a multiphase composite oxygen separation membrane.

2. Predictive models

The models presented in the following sections use geometric simplifications of the complex and random microstructures that are often found in real materials. The simplified systems allow the variations in the structure to be described with a statistical basis in a tractable manner, with the understanding that the results serve only as approximations for real microstructures. Specifically, the models are designed for composite systems consisting of two or more phases (with pores treated equivalently to a solid phase), composed of randomly distributed particle-like features of relatively uniform size and exhibiting long-range statistical homogeneity. This type of description applies to a number of materials which are fabricated by the mixing and pressing of various powders, followed by sintering at high temperature. During the sintering process, the powders densify to form the particle-like features considered in this work. Numerous researchers have also used a simulation approach to generate material microstructures by random packing of spherical particles within a volume, sometimes followed by a simulated sintering process [19–22]. It is realized that for most real materials, the concept of a “particle” is an abstraction, as neighboring features which are in close contact frequently form a contiguous network rather than an array of isolated particles. Understanding this distinction, it is assumed that these complex structures can still be represented approximately as an assembly of particles, some of which are in close contact with their neighbors due to the sintering process. For phases forming a contiguous structure, the terms “particle size” and “feature size” are thus used interchangeably. In addition to the references mentioned above, the idealization of real microstructures as random arrangements of particles of various phases has been used numerous times in the literature to develop analytical descriptions of device performance [23–26]. Certain features which may exist in real materials are not covered in this framework, including possible non-random agglomeration of particles of a certain phase, large disparities in structural/particle length scales, highly anisotropic features such as fibrous or planar structures, and graded structures. Therefore, the descriptions presented are not universally applicable, but rather apply to a certain class of particle-like materials. As a cubic RVE size is sought for each property, we introduce a convenient way to scale the size of the cube

$$L* = \frac{CubeEdgeLength\ [\mu\mathrm{m}]}{ParticleSize\ [\mu\mathrm{m}]} \tag{1}$$

The parameter L* provides a measure of the size of a cube by using the average number of particles per side as the measuring unit. The measure of average particle size is an approximation made by the researcher, and is meant to be a characteristic length of all particles/features in the microstructure.

2.1. Analytical model and results for the estimation of volume fraction RVE size

In this model, particles of various phases are assumed to be of constant size, randomly-located, independent, and densely packed. In reality, close contact and sintering between neighboring particles may create interconnections of somewhat smaller size than the “particles” themselves. However, in the evaluation of volume fraction, it is acknowledged that most of the material volume of a given phase is contained in the “particles” themselves rather than these tenuous connections. Therefore, sintered regions of varying (smaller) size than the constituent particles are not explicitly considered. While these are substantial simplifications, they allow for the development of a model when little is known about a real

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