Materials Characterization 140 (2018) 265–274

Contents lists available at ScienceDirect

Materials Characterization

journal homepage: www.elsevier.com/locate/matchar

Direct extraction of spatial correlation functions from limited x-ray tomography data for microstructural quantification

Hechao Li[a], Somya Singh[b], Nikhilesh Chawla[b], Yang Jiao[b,*]

[a] Mechanical Engineering, Arizona State University, Tempe, AZ 85287, United States
[b] Materials Science and Engineering, Arizona State University, Tempe, AZ 85287, United States

ARTICLE INFO

Keywords:
Microstructural quantification
Limited x-ray tomography data
Fourier slice theorem
Probability map
Correlation functions

ABSTRACT

Accurately quantifying the microstructure of a heterogeneous material is crucial to establishing quantitative structure-property relations for material optimization and design. There is a preponderance of previous work focused on structural quantification based on 2D images and reconstructed 3D volumes obtained via different imaging techniques. Here, we introduce novel procedures that allow one to extract key structural information in the form of spatial correlation functions from limited x-ray tomography data. In the case where only a very small number of x-ray tomographic radiographs (projections) are available, we derive a formalism based on the Fourier slice theorem to compute angularly averaged correlation functions directly from the radiographs. When a larger number of projections are available, we develop a procedure to extract full vector-based correlation functions. The key component of this procedure is the computation of a "probability map," which provides the probability of an arbitrary point in the material system belonging to a specific phase, via inverse superposition of the scaled attenuation intensities available in the tomography projections. The correlation functions of interest are then computed based on their corresponding probability interpretations from the probability map. The utilities of both of our procedures are demonstrated by obtaining lower-order correlation functions (including both the standard two-point correlation functions and non-standard surface functions) for a tin-clay composite material from both parallel-beam (synchrotron) and cone-beam (lab-scale) x-ray tomography projection data sets. Our procedure directly transforms the key morphological information contained in limited x-ray tomography projections to a more efficient, understandable, and usable form.

1. Introduction

The behavior and performance of an engineering material strongly depends on its complex microstructures over multiple length scales [1–3]. Recent developments in advanced imaging techniques such as x-ray tomography allow one to reveal detailed morphological features with sub-micrometer resolution and to investigate microstructural evolution in situ under different external stimuli [4–9]. Accurately quantifying the microstructure of a heterogeneous material from available image data is crucial to establishing quantitative structure-property relations for material optimization and design [10–20]. To this end, several classes of structure quantification schemes have been developed.

A widely used class of quantification schemes employs feature-specific statistics. In these schemes, the morphological features of interest are prescribed, which may include the shape and size of grains or precipitates [21–23], degree of connectivity of filamentary structures [24], degree of clustering of reinforcement particles [25], grain boundary misorientations [26], to name but a few. Accordingly, feature-specific statistics are employed to quantify the prescribed structural characteristics. For example, distribution of aspect ratios, effective radius and geometrical moments are usually utilized to quantify the grain morphology of a polycrystalline material [21]; while the coefficients of variation of local near statistics (e.g., nearest neighbor distance) are widely used to quantify the degree of clustering in particle reinforced composites [27]. Usually such structural statistics are highly system specific and generally cannot be utilized to quantify a generic microstructure. Another commonly used class of schemes borrows the techniques developed in computational pattern recognition. Specifically, a given microstructure image is decomposed (typically in Fourier space) and then is approximated and represented by weighted combination of a set of "basis" [28–32]. These pattern-recognition based methods are generic and can be easily applied to any microstructure on any length scale. However, the "basis" images usually contain random patterns without clear physical interpretations. In addition, a class of entropic descriptors has been developed, which identifies distinct local

* Corresponding author.
E-mail address: yang.jiao.2@asu.edu (Y. Jiao).

https://doi.org/10.1016/j.matchar.2018.04.020
Received 21 March 2018; Received in revised form 13 April 2018; Accepted 13 April 2018
Available online 14 April 2018

features on various length scales in a random microstructure and quantifies the frequency of occurrence of different local features for material characterization and reconstruction [33–35].

Recently, a new structure quantification scheme based on spatial correlation functions has been developed and successfully applied to model complex material microstructures on different length scales [17,24,36–51]. The spatial correlation functions are morphological descriptors that statistically characterize different geometrical and topological features of the materials of interest [3]. For example, the standard n-point correlation function $S_n(x_1, \ldots, x_n)$ gives the probability of finding a specific n-point configuration with all points x_1, …, x_n fall into the phase of interests (see Section 2 for a detail discussion). There are a number of advantages of correlation function-based quantification scheme: (i) The correlation functions such as S_n are generic but still possess clear physical interpretations. Certain feature-specific statistics such as average particle sizes can be directly extracted from the correlation functions. (ii) These statistically descriptors naturally arise in rigorous structure-property relations and be directly used to predict material properties for a given microstructure. (iii) Virtual 3D microstructures can be easily reconstructed from given correlation functions [17,29,41–43,52–71]. Recently, a novel hierarchical material informatics framework has been developed incorporating the high-dimensional structural data sets corresponding to generic spatial correlation function space [72–77].

Although very successful, the preponderance of previous work focuses on structural quantification based on 2D or 3D material images obtained via different imaging techniques. In the case of x-ray tomography microscopy, tedious segmentations of a grayscale reconstruction of attenuation coefficient map, obtained from filtered-back-projection (FBP) [78] or algebraic reconstruction technique (ART) [79], are required for resolving detailed microstructural features of different phases. Recently, several efficient "discrete tomography" techniques have been developed [80–88], which allow one to directly render 3D virtual material for subsequent analysis. Nonetheless, it is highly desirable to obtain morphological information directly from the raw x-ray tomography data for microstructure quantification, without explicit 3D material reconstruction.

In this paper, we present novel procedures that allow one to directly extract key structural information in forms of spatial correlation functions from limited x-ray tomography data. In the case where only a very small number of x-ray tomographic radiographs (projections) are available, we derive a formalism based on the Fourier slice theorem to compute angularly averaged correlation functions directly from the radiographs. When a larger number of projections are available, we develop a procedure to extract full vector-based correlation functions. The key component of the latter procedure is the computation of a "probability map", which provides the probability of an arbitrary point in the material system belonging to the specific phase of interest. Such a probability map can be computed via inverse superposition (i.e., taking arithmetic average) of the properly scaled attenuation intensities available in the tomography projections. The correlation functions of interest are then computed from the probability map, based on their probability interpretations. The utilities of our procedures are demonstrated by obtaining lower-order correlation functions (including both the standard n-point correlation functions and non-standard surface functions) for a heterogeneous material with tin spheres in a clay matrix. Both parallel-beam (synchrotron) and cone-beam (lab-scale) x-ray tomography projection data sets are used to compute the correlation functions. Our procedure directly transforms the key morphological information contained in limited x-ray tomography projections to a more understandable and usable form and opens new avenues for utilizing limited tomography data.

The rest of the paper is organized as follows: In Section 2, we provide fundamental definitions of the correlation functions employed in this work. In Section 3, we describe the procedure for directly extracting angularly average correlation functions from very limited x-ray tomographic data using Fourier slice theorem (i.e., the "Fourier-slice" approach). In Section 4, we respectively describe the method for computing the probability map and obtaining correlation functions from the corresponding probability map (i.e., the "probability-map" approach). In Section 5, we employ the both procedures to quantify a tin-sphere-clay microstructure form both limited synchrotron and lab-scale data sets. Concluding remarks are provided in Section 6.

2. Definition of Correlation Functions

2.1. Standard n-point Correlation Function

In general, the microstructure of a heterogeneous material can be determined by specifying the indicator functions associated with all of the individual phases of the material [3]. Without loss of generality, we focus on two-phase materials (binary medium) in this work. The generalization of the subsequent discussion to a multiple-phase system is straightforward.

Consider a two-phase heterogeneous material with volume V in either two- or three-dimensional space. This material contains two disjoint phase regions: phase 1 denoted by set V_1 with volume fraction φ_1, and phase 2 denoted by set V_2 with volume fraction φ_2. Based on the nature of the two-phase material, it is clear that $V_1 \cup V_2 = V$ and $V_1 \cap V_2 = 0$. In the following discussions, we consider phase 1 as our phase of interest, and the indicator function $I^{(1)}(x)$ of phase 1 is given by

$$I^{(1)}(\boldsymbol{x}) = \begin{cases} 1, \boldsymbol{x} \in V_1 \\ 0, \boldsymbol{x} \in V_2 \end{cases} \tag{1}$$

The indicator function $I^{(2)}(x)$ for phase 2 can be defined in a similar fashion, and it is obvious that

$$I^{(1)}(\boldsymbol{x}) + I^{(2)}(\boldsymbol{x}) = 1 \tag{2}$$

The n-point correlation function (or n-point probability function) $S_n{}^{(1)}$ for phase 1 is then defined as:

$$S_n^{(1)}(\boldsymbol{x_1}, \boldsymbol{x_2}, \ldots, \boldsymbol{x_n}) = \langle I^{(1)}(\boldsymbol{x_1}) I^{(1)}(\boldsymbol{x_2}) \ldots I^{(1)}(\boldsymbol{x_n}) \rangle \tag{3}$$

where the angular brackets "<…>" denote ensemble averaging over independent realizations of the random material. The two-point correlation (probability) function $S_2{}^{(1)}$ can be directly derived from Eq. (3), i.e.,

$$S_2^{(1)}(\boldsymbol{x_1}, \boldsymbol{x_2}) = \langle I^{(1)}(\boldsymbol{x_1}) I^{(1)}(\boldsymbol{x_2}) \rangle \tag{4}$$

If the material system is statistically homogeneous, i.e., the joint probability distributions describing the random microstructure are invariant under a translation (shift) of the space origin, $S_2{}^{(1)}$ is a function of the relative displacements, i.e.,

$$S_2^{(1)}(\boldsymbol{x_1}, \boldsymbol{x_2}) = S_2^{(1)}(\boldsymbol{x_2} - \boldsymbol{x_1}) = S_2^{(1)}(\boldsymbol{r}) \tag{5}$$

where $\boldsymbol{r} = \boldsymbol{x_2} - \boldsymbol{x_1}$. If the material system is further statistically isotropic, i.e., the joint probability distributions for the microstructure are invariant under rigid-body rotation of the spatial coordinates, $S_2{}^{(1)}$ becomes a radial function, depending only on the scalar separation distances,

$$S_2^{(1)}(\boldsymbol{x_1}, \boldsymbol{x_2}) = S_2^{(1)}(|\boldsymbol{r}|) = S_2^{(1)}(r) \tag{6}$$

In the ensuing discussions, we will drop the superscript denoting the phase index in $S_2{}^{(1)}$ for simplicity. Without further elaboration, S_2 always denotes the two-point correlation function for the phase of interest. Based on its definition, we can easily obtain the limiting values of S_2, i.e.,

$$\lim_{r \to 0} S_2(r) = \varphi_1 \text{ and } \lim_{r \to \infty} S_2(r) = \varphi_1^2 \tag{7}$$

Eq. (7) can also be derived from the probability interpretation of S_2, i.e., the probability of two random chosen points separate by distance r, both falling into the phase of interest. In general, the n-point correlation