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Reconstruction of heterogeneous materials via stochastic optimization of limited-angle X-ray tomographic projections

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X-ray tomography has provided a non-destructive means for microstructure characterization in three and four dimensions. A stochastic procedure to accurately reconstruct material microstructure from limited-angle X-ray tomographic projections is presented and its utility is demonstrated by reconstructing a variety of distinct heterogeneous materials and elucidating the information content of different projection data sets. A small number of projections (e.g. 20–40) are necessary for accurate reconstructions via the stochastic procedure, indicating its high efficiency in using limited structural information.

Keywords: Stochastic reconstruction; Material microstructure; Limited-angle projections; X-ray tomography

The physical properties and performance of heterogeneous materials are determined by their complex microstructures and how such microstructures evolve under various conditions [1,2]. Traditionally, the study of material microstructure has been limited by two dimensional (2-D) imaging techniques. Advances in experimental methods, analytical techniques and computational approaches have now enabled the development of 3-D analyses [3]. The study of 3-D microstructures under an external stimulus (e.g. stress, temperature and environment) as a function of time (i.e. 4-D materials science) is also particularly exciting.

X-ray tomography is an extremely attractive, non-destructive technique for characterizing microstructure in three and four dimensions [4–6]. In X-ray tomography, 2-D projections are usually obtained at small angular increments. Given a sufficiently large number of such 2-D projections, tomographic reconstruction techniques such as the filtered back-projection algorithm [7], algebraic reconstruction techniques [8] and the trajectory-based direct iterative reconstruction method [9] can be employed to generate a grayscale image of the microstructure. Further segmentation and thresholding analysis are used to resolve details of individual material phases and produce accurate digital representations of the 3-D microstructure. Such data sets can be used to quantify the microstructure and/or can be used as an input for microstructure-based modeling. Thus, X-ray tomography is an excellent technique that eliminates destructive cross-sectioning, and allows for superior resolution and image quality with minimal sample preparation [10–16].

The large number of 2-D projections required for traditional reconstruction algorithms strongly limits the application of this technique in 4-D materials science. An extremely large volume of data is usually needed as the input for the reconstruction algorithms, even for a single "snapshot" of the microstructure at a given time step. Characterizing an entire microstructural evolution process, at multiple time steps, may lead to hundreds of terabytes of data. Efficiently storing, retrieving and maintaining such large data streams are a significant challenge to the materials community. Therefore, it is highly desirable to devise alternative reconstruction procedures that can render accurate virtual microstructures from only a handful of 2-D projections.

If the material of interest contains only a small number of distinct phases and the phase properties (i.e. the attenuation coefficients) are known a priori (the focus of this paper), the reconstruction problem amounts to distributing different phases in a predefined discrete regular grid (e.g. simple cubic lattice), which is the focus of discrete

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tomography [17,18]. Discrete tomography is closely related to several other mathematical fields, including number theory [19,20], discrete geometry [21,22] and combinatorics [23,24]. It typically deals with reconstructions from a small number of projections, and several associated algorithms have been devised. For example, the discrete algebraic reconstruction technique (DART) [25,26] employs iterative segmentation of grayscale reconstructions to improve the accuracy for interface regions. The generic iterative methods [27] generally update a reconstruction for each projection angle separately, and thus the convergence and accuracy of the reconstruction depends on the angle selection schemes. In addition, a stochastic method [28,29] has been devised to improve the quality of pre-reconstructed grain maps.

Here, we present a stochastic optimization procedure to generate efficient and accurate reconstructions of heterogeneous material microstructures from limited-angle absorption contrast X-ray projections (i.e. limited tomography data). Our procedure is unique from previous discrete tomography reconstruction methods in several aspects: (i) no segmentation is needed in any stages of the reconstruction (in contrast to DART); (ii) projections of all angles are simultaneously considered and angle selections do not affect the convergence of the reconstruction (in contrast to the generic iterative methods); and (iii) reconstructions both from scratch (random initial microstructure) and from pre-reconstructed structures can be generated. We demonstrate the utility of our procedure by applying it to reconstruct a variety of material microstructures in two and three dimensions and to quantitatively examine the information content of a given tomography data set. We find that highly accurate reconstructions can be obtained using only 20–40 projections for the systems that we consider here. This suggests that the typical tomography data set that includes thousands of projections for a single microstructure may contain redundant structural information that can be possibly reduced to a much smaller minimal set without losing the accuracy in reconstruction compared to those obtained from the larger data sets.

We explain our reconstruction procedure by considering a 2-D binary material and the associated tomography data sets (i.e. projections) that are obtained using 2-D parallel beam geometry. However, our procedure is general and can be applied to multiple phase materials and other projection geometries. As schematically shown in Figure 1, parallel rays are sent through a material and a detector behind the material can register the intensity of the rays passing through the sample. If we denote the position of a ray at the detector by r for the projection associated with angle θ, the total attenuation of the ray $p(r, \theta)$ due to absorption is given by

$$p(r,\theta) = \ln(J/J_0) = -\int \mu(x,y)ds \tag{1}$$

where J_0 and J are the intensity of the incident and attenuated ray, respectively, and

$$\mu(x,y) = \mu_1 I^{(1)}(x,y) + \mu_2 I^{(2)}(x,y) \tag{2}$$

Here, μ_i is the attenuation coefficient of phase i and $I^{(i)}$ is the indicator function of phase i, which is equal to 1 if the point is in phase i and equal to 0 otherwise, i.e.

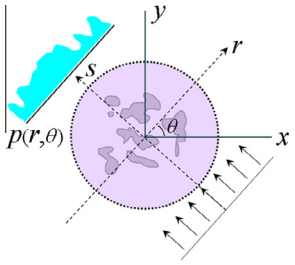

Figure 1. A schematic illustration of a parallel-beam tomography system. The incident rays are parallel to one another and are attenuated as they pass through the material sample. The intensity of the attenuated rays is obtained using a detector, from which the total attenuation $p(r, \theta)$ can be computed. This figure schematically shows a profile of the total attenuation associated with angle θ.

$$I^{(i)}(x,y) = \begin{cases} 1 & (x,y) \in V^{(i)} \\ 0 & \text{otherwise} \end{cases} \tag{3}$$

It can be seen that the phase indicator functions completely specify the material microstructure [1]. Thus, the goal of tomography reconstruction is to recover the phase indictor functions $I^{(i)}$ from the total attenuation (i.e. the projections) at different angles $p(r,\theta)$.

Our reconstruction procedure is inspired by the stochastic optimization scheme developed by Yeong and Torquato to generate virtual microstructures from prescribed statistical morphological descriptors of the microstructure, i.e. various correlation functions [30–33]. Given a prescribed set of tomographic projections (i.e. a set of total attenuation values at prescribed angles $p(r,\theta)$), a trial binary microstructure is randomly generated (e.g. by assigning a phase to a pixel with certain probability). The attenuations values $p(r,\theta)$ associated with the trial microstructure at corresponding angles are then computed. We define an energy functional E associated with the trial microstructure, which is the sum of the squared difference between the prescribed (p^*) and trial attenuation (p) values, i.e.

$$E = \sum_{\theta}\sum_{r}[p(r,\theta) - p^*(r,\theta)]^2 \tag{4}$$

Thus, the reconstruction problem is formulated as an energy minimization problem in which the trivial microstructure evolves in order to lower the associated energy E. Ideally, the "ground-state" trial microstructure, i.e. the one with $E = 0$, possesses a set of total attenuations that is identical to the actual microstructure. Such a "ground-state" structure is considered to be the reconstruction of the actual microstructure.

The energy minimization problem is solved using a simulated annealing procedure [34]. Specifically, given an old (or initial) trial microstructure (with an energy E_{old}), a new trial microstructure is generated by changing a randomly selected pixel of phase i to phase j ($i \neq j$), or by switching the position of two randomly chosen pixels belonging to different phases. The former operation is to change the volume fraction of the phases while the latter is to redistribute the phases to change the morphology of the trial microstructure. After a new trial microstructure is generated, its energy E_{new} is computed using Eq. (4). The probability that this new trial microstructure will