

A DATA-CONSTRAINED COMPUTATIONAL MODEL FOR MORPHOLOGY STRUCTURES

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ABSTRACT

A data-constrained computational model has been developed for generation of a microscopic 3D morphology structural map of a material sample, using 3D sets of CT-reconstructed tomograms and a limited number of 2D morphological section maps. The model is defined on a 3D hyper-cubic lattice. Each voxel of the lattice represents an elementary volume of material. It is assumed that the morphological sections are representations of the 3D morphology structure and that the material composition of a given voxel is determined statistically by its neighbouring voxels. Efficient computational algorithms have been developed which incorporate the sum rules of total volume-fractions and the total linear-absorption coefficients on each voxel. The model algorithms have been implemented as a user-friendly MS-Windows software package. The software generated morphology structures agree reasonably well with the actual structures for a range of simulated testing data sets. Our approach to 3D compositional morphology structures has a number of advantages in materials design and modelling. For example the 3D morphology maps can be used for microscopic chemical processes modelling on a real representation rather than an idealized one.

KEYWORDS: Data-constrained, computational model, micro-morphology, cellular automata, tomography, linear-absorption coefficients, statistical mechanics, information theory.

INTRODUCTION

Materials design is entering a new era with the prospect of building materials from fundamental atomic or molecular building blocks. One of the principal challenges facing nano-engineering is characterization of micro-morphology structures. Complexity of morphology arises from the combination of simple subunits by uncertain mechanisms into unknown forms. Therefore, structural characterization is key not only in understanding the resultant morphology but also the mechanistics of its formation. Structure-property relationships of materials have been of interest for many years, but researches in the early part of the twentieth century were limited by the availability of techniques capable of probing materials down to the microscopic length scale. Advances of computer technology has had a big impact on materials characterization since modern materials characterizations often involve the collection of huge amounts of data such as images with spectra associated with every pixel – the so-called data cubes.

There has been a steady advancement in theoretical and numerical modeling of material micro-structures [1-2]. Those models are particularly successful in simulating the formation and structures of grains on fine length scales. Nevertheless, in most cases, comparisons between model predictions and experiments could only be made statistically. That is,

the model-predicted micro-morphology structures would not be suitable for detailed comparisons with specific experimental samples.

There is a wealth of experimental techniques to provide elemental, chemical, topological, morphological, and structural information about many types of materials and numerous books have been published on specific methods. For routine use, many of these techniques are often either too time consuming, costly, or are only capable of probing material samples on or near their surfaces. Detailed 3D micro-morphology structural information is often obtained using destructive processes, such as ion beam etching, in combination with surface sensitive methods. What is desirable is a non-destructive technique that allows the determination 3D physical and chemical morphology.

At present there have been significant advances in the computation of material properties and of processes that occur in materials. Rather than modeling on a statistical basis or by assuming average processes, it is now possible to simulate materials processes in structures. This approach could lead to a great increase in accuracy particularly of structures which show significant local variations in properties, such as the diffusion of ionic materials through a porous structure. The rate of diffusion will be significantly influenced by the interaction of the ionic species with

the surface charge on the pore walls which will be controlled by pore size, local surface charge density, pore liquid conductivity and pH. All these factors will vary significantly through a real structure. If a realistic 3D model of the porous material can be developed, an accurate simulation of diffusion that incorporates the effect of variation in properties could be determined. This could then be verified using the actual structure and the sensitivity of materials variations examined using the simulation. Such an approach could lead to rapid improvements in design of materials with complex functionality

Computerized tomography (CT) has been widely adopted in the study of materials micro-structures non-invasively [3]. With CT, a material sample is scanned by an x-ray or other particle beam such as electrons or neutrons. The transmitted or diffracted beam is detected which is then used to construct a 3D image of the sample. Compositional or morphological structures could be derived from the 3D images under certain conditions [4-5]. The techniques have limited success when different material compositions exhibit similar absorption or diffraction characteristics, or when the CT resolution is insufficient to resolve the fine structures.

There are, however, areas where the combination of computational modeling and experimental techniques can make a further impact. For example a 3D tomography scan in principle could be combined with 2D elemental or chemical mapping to produce 3D chemical compositional structures. That is, a detailed 3D morphological structure could be obtained through taking 3D linear-absorption tomography maps of samples and combining this information with a limited number of 2D elemental chemical maps, and extrapolating the composition of the sample throughout the sample volume.

In this paper, we will present our effort in data-constrained morphology (DCM) computational modeling. The approach incorporates 3D sets of CT reconstructed tomograms, a limited number of 2D surface and sectional morphology maps, and the known parameters of the material compositions. The tomograms, sectional maps and the material parameters are used as constraints for our DCM computational model. Our approach allows detailed sample-specific comparisons between the model-predicted morphology structures and experimental measurements. Sample-specific bulk material properties would be derived from the predicted morphological structures, as shown in Figure 1.

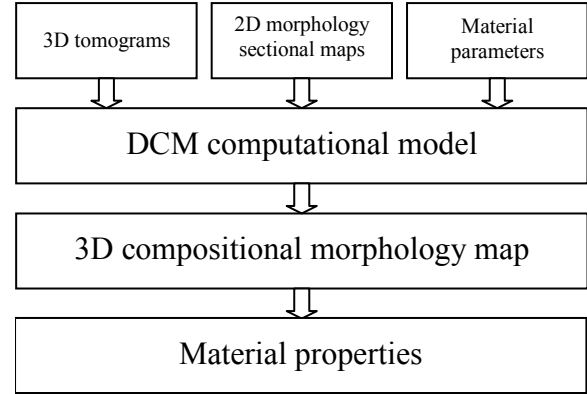


Figure 1: Data-constrained morphology modeling.

DATA-CONSTRAINED MORPHOLOGY MODELLING

The model is conveniently defined on a 3D simple cubic lattice. Each site of the lattice is represented numerically by a voxel (volume pixel) [6-9]. Each voxel contains $M + 1$ volume-fraction channels where M is the number of compositions of the material sample. The 1st channel is for the void volume-fraction. The void represents the vacant spaces in a material. The remaining volume-fraction channels represent the volume-fractions of the M compositions. It also contains L total linear-absorption coefficients [10] channels where L is the number of 3D sets of CT reconstructed tomograms for a material sample. For x-ray tomography, different sets of tomograms can be taken with different x-ray wave lengths. The same principle applies to other type of tomography techniques. For instance, multiple sets of tomograms can be produced by using different particle energies for electron or neutron tomography.

The values of the channels define the state of a voxel. It is obvious that each voxel can take an infinite number of possible states. By definition, the volume-fraction of a material composition can only take a value in $(0, 1)$ and the total volume-fractions in a voxel must add to one; and an absorption coefficient cannot take a negative value. It is known, to a good approximation, that the total linear-absorption coefficient is additive [10]. Consequently, we have

$$\left\{ \begin{array}{l} 0 \leq v_{\alpha,i} \leq 1; \alpha = 0, 1, \dots, M \\ \sum_{\alpha=0}^M v_{\alpha,i} = 1 \\ \bar{\mu}_i(\lambda) = \sum_{\alpha=0}^M v_{\alpha,i} \mu_{\alpha}(\lambda); \\ \lambda = \lambda_1, \lambda_2, \dots, \lambda_L \end{array} \right. \quad i = 1, 2, \dots, N \quad (1)$$

where α denotes the compositions; i is the position index of a voxel, $v_{\alpha,i}$ is the volume-fraction of the α 'th composition at location i ; for an x-ray wave length or particle energy λ , $\bar{\mu}_i(\lambda)$ is the total linear-absorption coefficient of the i 'th voxel and $\mu_\alpha(\lambda)$ is the total linear-absorption coefficient for the α 'th composition; and N is the total number of voxels. The values for $\bar{\mu}_i(\lambda)$ are derived from the appropriate tomograms. In the 3rd formula above, an implicit assumption has been made that the voxel sizes are small such that the total absorption or diffraction by a voxel is equivalent to that of a random mixture of compositions.

The purpose of the data-constrained morphology modeling is to construct a material microstructure represented by the channel volume-fractions $v_{\alpha,i}$ for each voxel as defined above. Equation (1) forms part of the constraints to the model. For a case with $L \geq M$, equation (1) alone could lead to a unique solution to the problem. For cases with $L < M$ or where the number of independent equations derived from the 3rd formula in Equation (1) is less than M , Equation (1) serves as a constraint which defines a narrowed solution space.

For a voxel whose numerical state cannot be determined uniquely by Equation (1), it is assumed that its state (within the constraints defined by Equation (1)) is determined statistically by its neighbors. That is, the model is a data-constrained probabilistic cellular automaton [11-13].

The model also accommodates sections and regions with known morphology structures from experimental measurements. Those sections and regions constitute additional constraints to the solution. The probability of the neighboring influence is assumed to be governed by the information theory and the Boltzmann distribution [14]. In combination with measured sectional morphology maps, the assumption enables us to numerically derive the values of neighboring influence probabilities. In other words, within the solution space as defined in Equation (1), a complete 3D morphology structure is computed self-consistently. Such self-consistent computations will be implemented and will be the subjects for subsequent publications.

A software package, DCM (Data-Constrained Morphology), has been developed using CSIRO proprietary data-constrained modeling algorithms. It takes as input 3D sets of tomograms from appropriate

tomography techniques and a limited number of measured morphology sectional maps. The output from the software is a complete 3D morphology structure with volume-fraction values for each composition (including void) at each grid point.

Comparisons between the DCM software predicted morphology structure and the original data will be presented in the next section.

NUMERICAL RESULTS

In order to evaluate the model, two sets of simulated data have been generated. The data sets have a grid size of 100 by 100 by 30, and an 8-bit data resolution.

The 1st simulated data set contains one chemical composition (Chem A) plus the void ($M = 1$). The data set is generated by randomly filling a 100×100×30 voxel grid with cubical Chem A blocks of random sizes in (1, 20), using the following procedures:

- Start with a 100×100×30 voxel grid. Each voxel is allocated with 2 volume-fraction data channels (channels 0 and 1 for void and Chem A), and a tomography data channel (channel 3).
- Channel 0 is assigned a value 1 and other channels with a value 0 representing that the grid is initially occupied all by void.
- Compute the size of a cubic block using the formula $s = 1 + 19r^3$ where r is a random number in (0, 1). The random number is raised to power 3 to balance the relative weights for small and large blocks.
- Assign a volume-fraction value of $v = 0.1 + 0.9r$ to the block and place the block at a random location in the grid by expelling the space originally occupied by the void.
- If the total volume-fraction of Chem A at any voxel goes beyond 1, the value is scaled back to 1.
- Repeat 100 times the previous 3 steps.
- A 3D set of tomogram is calculated using the 3rd formula in Equation (1), assuming one x-ray or particle energy λ ($M = 1$). Without loss of generality, an arbitrary unit has been used so that $\mu_{\text{ChemA}}(\lambda) = 1$.
- The computed channel values are output as images on XY planes in 8-bit uncompressed TIFF format.

A set of 100×100 uncompressed TIFF images have been created for the XY cross-sections along the Z axis for the void, Chem A and the tomograms. The

sections 5, 15 and 25 along the Z-axis for the void and the Chem A channels are shown in Figure 2.

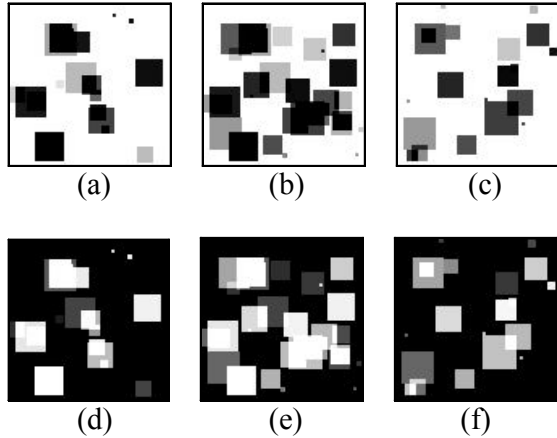


Figure 2: Sectional images of the void and the Chem A volume-fractions along the Z-axis for the simulated single composition system. The intensity (brightness) of a pixel represents the corresponding volume-fraction value. (a): Void volume-fractions at section 5. (b) Void volume-fractions at section 15. (c) Void volume-fractions at section 25. (d) Chem A volume-fractions at section 5. (e) Chem A volume-fractions at section 15. (f) Chem A volume-fractions at section 25.

The simulated 3D set of tomograms and sections 1, 10, 20 and 30 along the Z-axis for the Chem A are used as input data for the DCM software. Figure 3 shows the DCM software computed volume-fractions for the void and the Chem A channels on sections 5, 15 and 25. The figures show an excellent agreement between the original data and the DCM software predictions. This is expected for a case with $L = M$. On a DELL X300 MS-Windows XP notebook computer with a 1.4GHz Pentium M CPU and 1GB of RAM, it takes a total of 1.6 seconds of CPU time to complete the computation. For a different grid size, the CPU time is expected to be proportional to the grid size. For a large grid size, considerable amount of CPU time may be required. To a lesser extent, the CPU time may vary with different data sets depending on the structural details.

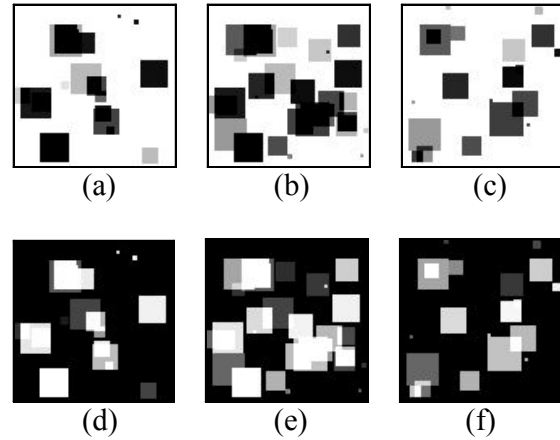


Figure 3: Sectional images of the void and the Chem A volume-fractions along the Z-axis for a single composition system predicted using the DCM software. The intensity (brightness) of a pixel represents the corresponding volume-fraction value. (a): Void volume-fractions at section 5. (b) Void volume-fractions at section 15. (c) Void volume-fractions at section 25. (d) Chem A volume-fractions at section 5. (e) Chem A volume-fractions at section 15. (f) Chem A volume-fractions at section 25.

Similar procedures have been used in the generation of another simulated data set which contains two chemical compositions (Chem A and Chem B) plus the void ($M = 2$). Another arbitrary unit has been used such that $\mu_{\text{ChemA}}(\lambda) = 1$ and $\mu_{\text{ChemB}}(\lambda) = 2$. A 3D set of tomograms is computed similarly using the 3rd formula in Equation (1), assuming one x-ray or particle energy λ ($L = 1$). The data set is again generated by randomly filling a $100 \times 100 \times 30$ voxel grid with Chem A and Chem B cubic blocks of random sizes in (1, 20) and random volume-fraction values. A similar volume-fraction scaling is used to ensure that the total volume-fraction at any grid point is less than or equal to one. A set of 100×100 uncompressed TIFF images have been created for the XY cross-sections along the Z axis for the void, Chem A, Chem B and the tomograms. The sections 5, 15 and 25 along the Z-axis for the void, Chem A and Chem B volume-fraction channels are shown in Figure 4.

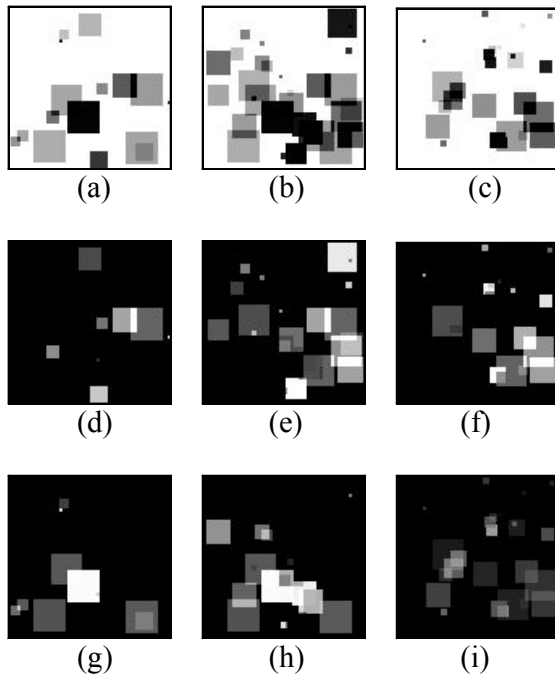


Figure 4: Sectional images of the void and the material composition volume-fractions channels along the Z-axis for the simulated two composition system. The intensity (brightness) of a pixel represents the corresponding volume-fraction value. (a): Void volume-fractions at section 5. (b) Void volume-fractions at section 15. (c) Void volume-fractions at section 25. (d) Chem A volume-fractions at section 5. (e) Chem A volume-fractions at section 15. (f) Chem A volume-fractions at section 25. (g) Chem B volume-fractions at section 5. (h) Chem B volume-fractions at section 15. (i) Chem B volume-fractions at section 25.

The simulated 3D set of tomograms and sections 1, 10, 20 and 30 along the Z-axis for the Chem A and Chem B are used as input data for the DCM software. Figure 5 shows the DCM software computed volume-fractions for the void, the Chem A and the Chem B on sections 5, 15 and 25. The figures show a reasonable agreement between the original data and the DCM software predictions. The apparent differences between the original and the predicted data should be due partly to the lack of a self-consistent computational algorithm in the current DCM software implementation, and partly due to the fact that the data set is generated with an arbitrary random process. The total CPU time was 2.5 seconds on the same DELL X300 notebook computer.

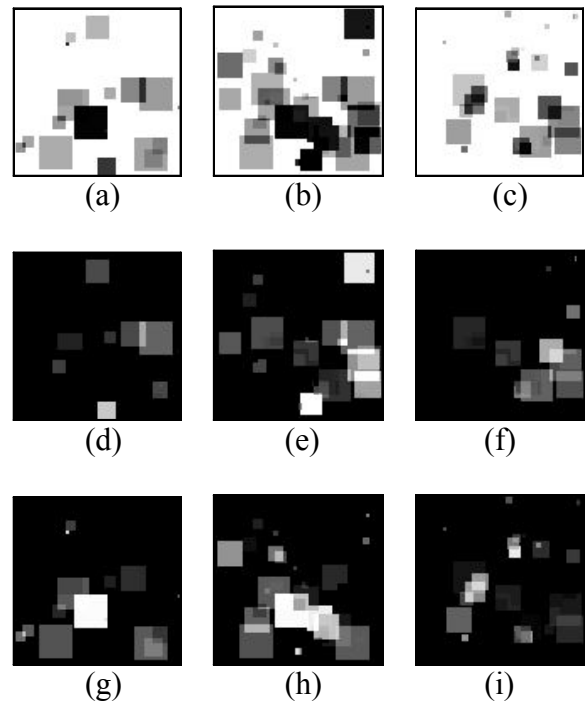


Figure 5: Sectional images of the void and the material composition volume-fraction channels along the Z-axis for the two compositions system predicted using the DCM software. The intensity (brightness) of a pixel represents the corresponding volume-fraction value. (a): Void volume-fractions at section 5. (b) Void volume-fractions at section 15. (c) Void volume-fractions at section 25. (d) Chem A volume-fractions at section 5. (e) Chem A volume-fractions at section 15. (f) Chem A volume-fractions at section 25. (g) Chem B volume-fractions at section 5. (h) Chem B volume-fractions at section 15. (i) Chem B volume-fractions at section 25.

SUMMARY

Knowledge of the material structures at atomic, nano and micro length scales is critical in understanding structure-properties relationships of materials. However, the available computational modeling techniques are inadequate to produce accurate sample-specific predictions; and it is time-consuming and expensive to probe the material structures experimentally at such length scales. This paper presents a data-constrained morphology (DCM) computational model for generation of detailed 3D morphology structure of a material using 3D sets of CT reconstructed tomograms and with a limited number of sectional morphology maps. The model is defined conveniently on a 3D cubic lattice. The model incorporates the sum rules for total volume-fractions and total linear-absorption coefficients, and takes a probabilistic cellular automata approach. The model has been implemented as a user-friendly software package incorporating CSIRO proprietary

data-constrained algorithms under the MS-Windows environment. The morphology-structures predicted using the software package agree reasonably well with the actual structures which have been simulated by random filling of a 3D grid with cubes of random sizes.

It is expected that errors between the original and the software predicted data would be larger as the distance is further away from the input sections. In comparing the original and the predicted data, we have selected the largest possible such distances. So Figures 4 and 5 should represent the largest discrepancies. Nevertheless, such errors are reasonably small as shown in the figures. Future advances of the model should lead to further improvement in prediction accuracy. Such advances will be incorporated in the future releases of the software package.

The model is generic in that it should work with different kinds of tomography techniques, such as x-ray, electron and neutron tomography. The software would be a valuable tool for material characterization and modeling. In progress are development and incorporation of the further analysis techniques, and testing and validation with more realistically simulated and experimental data sets. These will be the subjects of subsequent publications.

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