Solid Freeform Fabrication 2019: Proceedings of the 30th Annual International
Solid Freeform Fabrication Symposium – An Additive Manufacturing Conference

A Universal Material Template for Multiscale Design and Modeling of Additive Manufacturing Processes

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Abstract

In this paper, a universal material template is developed to digitally describe the materials with spatially distributed compositions and microstructures for multiscale design and modeling of additive manufacturing processes. The developed template is organized in the form of a multi-level hierarchical structure. The root node of a material template contains four sub-nodes. They are "descriptors list", "constituent materials", "position information" and "primitive information". The format of each sub-node has been given in this paper to help users to establish a standardized description of microstructures of materials. To validate the effectiveness of the proposed template, the microstructures of two different types of commonly used materials in additive manufacturing processes are reconstructed from the pre-defined material templates. The results show the developed material template can accurately and precisely control the microstructures of materials. Based on the developed material template, the multiscale heterogeneous modeling method can be developed in the future.

1 Introduction

Additive Manufacturing (AM) technologies provide great design freedom on the parts with both complex geometries and material distributions [1]. Both materials' compositions and microstructures can be spatially varied by carefully tuning the process parameters during the fabrication [2]. These AM fabricated heterogeneous objects can achieve superior performance especially in the applications where multifunctional requirements are simultaneously expected[3].

To digitally describe the heterogeneous object in a computer, both geometry and materials of the heterogeneous object need to be modeled. In general, the heterogeneous object modeling process can be divided into two portions: geometric modeling and material modeling. Among them, the geometric modeling process focuses on representing the geometry of a designed object, while the material modeling process is developed to describe the material distribution inside the object. According to the survey from Kou and Tan [4], the heterogeneous object model can be generally described by a fiber bundle $E^3 \times E^k$, where geometry space E^3 is the base space, the material space E^k is the fiber space. k is the number of constituent materials under the investigation. In the past, most heterogeneous modeling methods only focus on the material compositions, where the detailed microstructures of the material are not considered. This approach is only appropriate for those Functionally Graded Materials (FGMs) whose microstructures don't change spatially. When it comes to those heterogeneous materials with spatially varied microstructures, this type of heterogeneous modeling method is no longer effective.

To solve this problem, material descriptors were developed to quantitatively characterize the materials with stochastically distributed microstructures. These descriptors cannot only be used to describe material compositions but also are able to characterize the shape of the material's microstructure. For example, n-point correlation functions have been widely used to quantitively describe the distances between different phases [5]. These descriptors also have strong relations to the properties of materials. Some existing research shows two-point and three-point correlation function are closely correlated to the elastic stiffness of the materials [3], while strain localization and damage evolution are sensitive to the higher order of n-points correlation functions [4]. Besides n-point correlation functions, Minkowski functionals[6] are another type of descriptors that have been used to characterize the microstructure of materials. They have been successfully used to describe the particle-based materials as well as materials generated with randomized Voronoi tessellations [7]. In addition to that, Cumulative Distribution Functions (CDFs) [8, 9] have also been used as a type of material descriptor to directly describe the size or shape of microstructure. Particularly, the size or shape of stochastically distributed microstructures is characterized by a group of random variables whose CDFs are given. Compared to those material descriptors based on n-point correlation functions, CDFs have more clear physical meaning. They can be obtained from the Scanning Electron Microscope (SEM) or EBSD (Electron Back Scatter Diffraction) images of materials [10]. Moreover, they also enable the reconstruction of material microstructures. Several algorithms [9, 10] have been developed to reconstruct the microstructures of poly-crystal metals based on their CDFs.

Even though CDFs have some advantages compared with other material descriptors, it should be noticed that it is still difficult to parametrically describe CDFs spatially. Moreover, every specific type of materials has its own CDFs. Even for the same type of materials, different designers may use different CDFs to describe its microstructure. Thus, there is a barrier to data exchange and re-use. To solve these issues, a universal material template is developed in this paper. The developed material template aims to provide a universal standardized description of material microstructures. It has two unique capabilities. Firstly, the developed template can be applied to all types of materials including the materials with stochastic microstructures such as polycrystalline metals, short fiber-reinforced composites, and the materials with periodic or architectured microstructures, such as lattice or cellular materials. Secondly, based on the descriptors defined in a material template, a heterogeneous object can be accurately described. Based on the distribution of material descriptors, the microstructure of the heterogeneous object can be reconstructed for simulation or fabrication purposes.

The rest portion of this paper is organized as followed. In Section 2, the detailed structure of the developed material template will be introduced. Then, two examples will be presented in Section 3 to illustrate how the developed material template can be used to reconstruct the microstructure of the described materials. A short summary and future research directions will be concluded at the end of this paper.

2. Universal Material Template

The universal material template developed in this paper aims to provide a standardized procedural description of the mesoscale or microscale structures of materials. It is organized in a hierarchical manner and represented by a tree structure. The first level of this template is illustrated in Figure 1. Four sub-nodes are attached under the root node of the material template. These four sub-nodes will be introduced respectively in the following contents of this section.

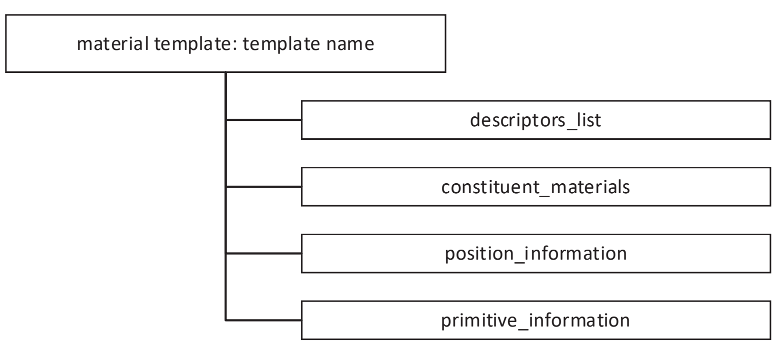


Figure 1 Material template: Level 1

2.1 Descriptors list

The first sub-node defined under the root node of a material template is "descriptors_list". Under this sub-node, the descriptors which are used to control the shape and size of material microstructures are defined. The Backus–Naur form (BNF) of this sub-node is defined as:

<descriptors_list>::=<descriptor_node>{,<descriptor_node>}
<descriptor_node>::= <descriptor_name> , <descriptor _type><descriptor_range>
<descriptor_name>::= <string>
<descriptor_type>::= "double"| "int"

The descriptors defined under this sub-node can be divided into two groups. The first group of descriptors is used to directly control the size and shape of material microstructures. For example, as shown in Figure 2, the cell size l_c and the strut dimension d are two descriptors defined under this sub-node of Body-Centered Cubic (BCC) lattice materials. By changing these two descriptors, designers can obtain a series of BCC lattice with different microstructures.

The second group of descriptors defined under this sub-node is used to control the probability distribution of the size and shape of material microstructures. This group of descriptors is mainly used for the materials consisting of stochastically distributed microstructures. The size and shape of these materials' microstructures are directly controlled by a series of random variables. The probability distributions of these random variables are controlled by these descriptors. For example, Figure 3 shows a "descriptors list" node of a short fiber-reinforced material. In this node, nine different descriptors are defined. Among these nine descriptors, only $\mathrm{v_f}$ is used to directly characterize the volume fraction of reinforced fibers. The other eight descriptors are used to control the Probability Density Function (PDF) of random variables. These eight descriptors can be further divided into four groups. Among them, descriptor $(\mu_\mathrm{d}, \sigma_d)$ is a group of descriptors used to describe the distribution of the fiber diameter. $(\mu_\theta, \sigma_\theta)$ and (μ_ϕ, σ_ϕ) are two groups of descriptors used to describe two random variables θ and ϕ. These two random variables are used to define the fiber orientation. The detailed discussion of these two random variables will be illustrated in sub-Section 2.2.4. The last group of descriptors $(\mu_\mathrm{r}, \sigma_r)$ is used to characterize the length distribution of fibers. Based on these eight descriptors, the fiber's orientation, length, and diameter can be fully described.

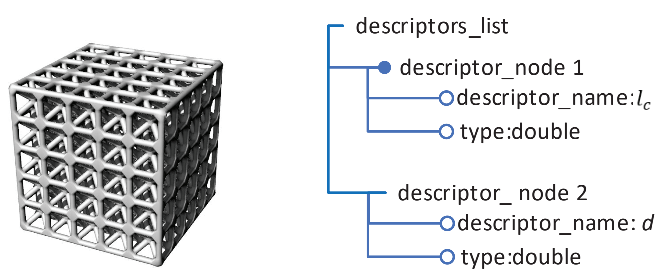
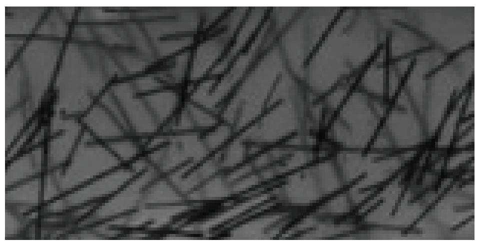
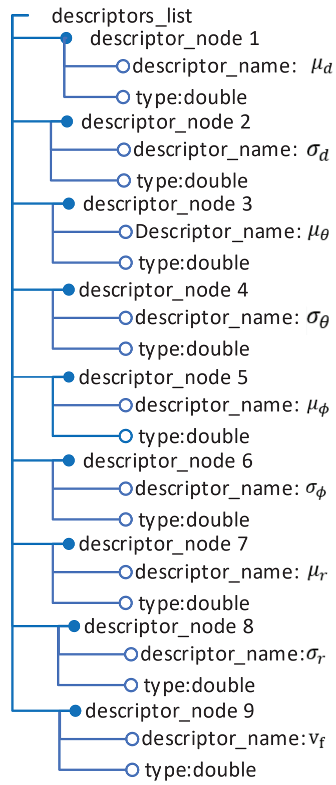


Figure 2 A "descriptors_list" node for BCC lattice



(a) short fiber reinforced composite



(b) "descriptors_list" node of short fiber reinforced composite

Figure 3 A "descriptors_list" of a short fiber reinforced material

2.2 Constituent materials

The second sub-node defined under the root node of a material template is the "constituent materials" node. Under this sub-node, all the constituents contained in the material's microstructure need to be described. The BNF definition of the "constituent_materials" node is provided as:

<constituent_materials>::=<material>{,<material >}
<material>::=<material_name>,<type>,[volume_fraction][,<template_name>,<values>]
<material_name >::= <string>
<type>::=inclusion|matrix
<volume_fraction>::=<double>|<descriptor>
<template_name>::=<string>
<values>::= <double>|<int>|<descriptor>{,<double>|<int>|<descriptor>}

Under the "constituent materials" node, "material" sub-nodes are defined to represent its material constituents. Each "material" node is described by a string representing its name. In general, material constituents described under the "constituent_materials" node can be classified into two groups: matrix and inclusion. In each material template, the number of matrix material constituents should be always smaller or equal to one, while there is no limitation on the number of inclusion material constituents. Only the shapes of inclusion materials are described under the "primitive information" sub-node of a material template. For those regions without inclusion materials, it assumed to be filled with the matrix material if the matrix material exists, otherwise, these regions will keep as voids. The example of the "constituent_materials" node of BCC lattice is given in Figure 4. In this type of material, there is no matrix constituent, only the inclusion material is described.

In addition to material type, the volume fraction of the material constituent is also necessary for some types of materials. For example, the volume fraction of the reinforced fibers needs to be defined for the short fiber-reinforced composite shown in Figure 3 (a). Its value can be controlled by the descriptor defined in the "descriptors_list" node. The example of "constituent materials" node of the short fiber reinforced materials is provided in Figure 5. In this example, the volume fraction of fibers is described by the descriptor v_f defined in the "descriptors_list" node shown in Figure 3 (b)

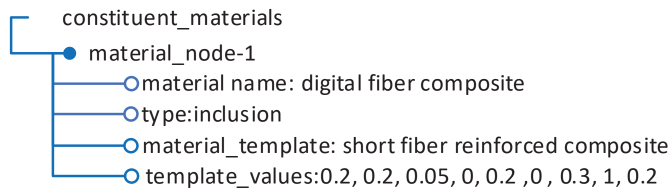


Figure 4 The "constituent materials" node of BCC lattice

It should be noted that the constituent material defined in the template can be described further by the material template and the value of its associated descriptors defined on the lower scale. For example, in Figure 4, we have a BCC lattice template whose lattice struts are made of the short fiber-reinforced composite. Thus, the template name and its corresponding descriptors' values are attached under the "material" node of BCC lattice.

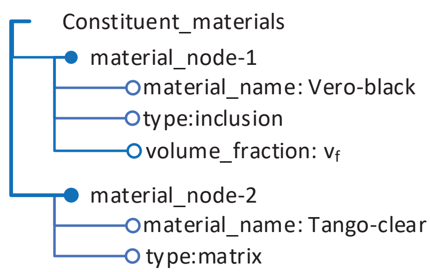


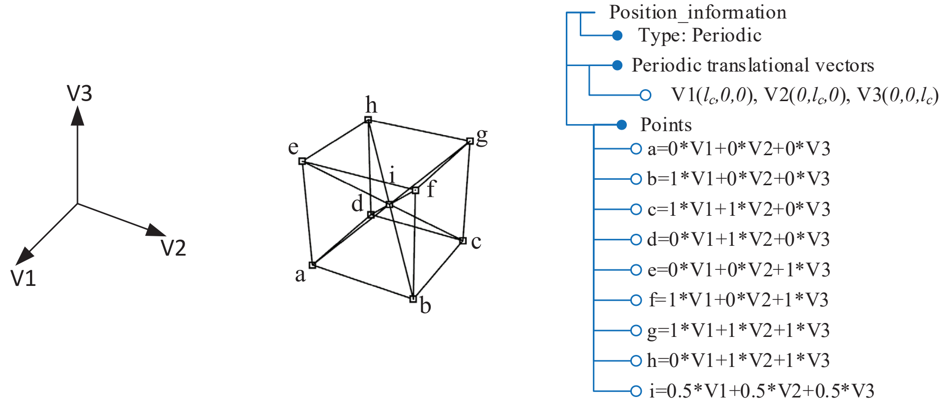
Figure 5 The "constituent materials" node of short fiber-reinforced composite

2.3 Position Information

To describe the relative positions of the primitives of material microstructures, the "position information" node is defined. The BNF description of the position information node is expressed as:

<position_information>::=<type>,[translational_vectors],<points>
<type> = periodic | stochastic
<translational_vectors>::=<vector_name>(<vector>,<vector> [,vector])
<vector>::=<coordinate>
<coordinate>::=(<double>,<double>,<double>)|<coordinate_expression>
<coordinate_expression>::=<double>*<vector_name>{+|-<double>*<vector_name>}
<points>::=<point>{,<point>}
<point>::=<point_name>,<coordinate>,[position parameters]

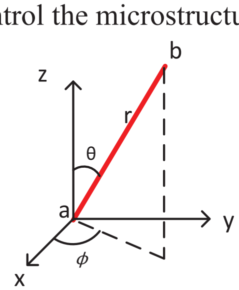
Several terms in this description are complicated and are explained using the lattice materials and short fiber-reinforced composite as examples below. In Figure 6, an example is provided to illustrate how to define the position information of BCC lattice materials. Since this type of material consists of periodic microstructures, the periodic translational vectors need to be defined under this node. Particularly for this example, three translational vectors are defined. The coordinates of these vectors are provided. Besides translational vectors, nine points are also defined under the "points" sub-node. These nine points can be used to describe the position of primitives inside the microstructure of a material. The coordinates of these nine points are described by the coordinate expressions which are defined based on the translational vectors.



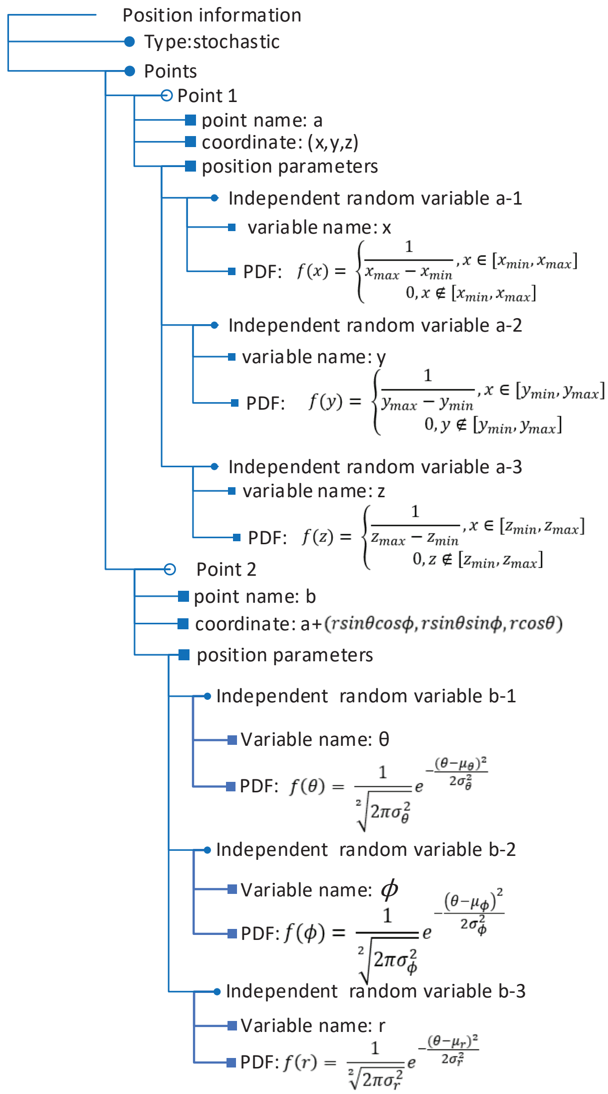
(a) Periodic translational vector of BCC lattice and its unit cell (b) Position information of BCC lattice

Figure 6 "Position information" node of BCC lattice structures

Besides the materials with periodic microstructures, those materials with stochastic microstructures can also be described by the developed material template. An example of the "position information" node of a short fiber reinforced material is given in Figure 7. Under this node, there are two sub-nodes: "type" and "points". Since the fiber is randomly distributed inside the matrix material, the points defined under this node are stochastically distributed. Thus, the attribute of "type" sub-node is set as "stochastic". As to the sub-node of "points", there are two points defined under this sub-node. These two points refer to as the start and end point of a fiber. Among these two points, the start point a is called an independent node. Its position is described by three independent random variables: x, y, and z. To characterize the value of these three random variables, the PDFs of these three random variables are attached to the sub-node called "position parameters". For this example, these three random variables all follow the uniform distribution. Another point defined under the "points" node is the end of a fiber. Unlike the start point a, the end point b is a dependant point. Its position is controlled by the independent node which is the start point of the fiber in this example, as well as a set of related random variables. The relationship between the end point and the start point of the fiber is graphically described in Figure 7 (a). In this figure, θ, ϕ and r are three random variables whose PDFs are given under the "position parameters" sub-node. In these PDFs, six material descriptors are used to control the PDFs of these random variables. Thus, these six material descriptors can be used to further control the microstructures of materials.



(a) The position and orientation of a fiber



(b) “position information” node

Figure 7 “position information” node of short fiber-reinforced composite

2.4 Primitive Information

The last sub-node under the root node of a material template is called “primitive information”. This node records the information related to the shape of primitives included in the microstructure of the defined material.

In order to describe a variety of shapes of material’s primitives, a hybrid modeling method is used which integrates the Constructive Solid Geometry (CSG) modeling method with an implicit modeling method. Particularly, the shape of a material primitive can be described procedurally by decomposing a complex primitive shape into a combination of simple geometry elements. Geometric operations, such as Boolean operations, are defined between these simple geometry elements to describe their relations and the final geometry of the material primitive. As to those simple geometric elements, implicit functions can be constructed to parametrically control their shapes. By changing the parameters defined in the implicit functions of geometric elements, designers can precisely and parametrically control the shape of the material’s microstructure. The proposed method enables great freedom to parametrically describe a wide range of material microstructures. To formalize the description of the "primitive information" node, its BNF formulation is given:

<primitive_information>::= <primitive>| {,<primitive>}

<primitive> ::=<primitive_name>,<material_information>,<sub_primitive>

<sub_primitive>::= <element>|(<sub_primitive> <operation> <sub_primitive> {<operation> <sub_primitive>})

<element> ::= <implicit_function>,<function_parameters>

<function_parameters>::=<function_parameter>{,<function_parameter>}

<function_parameter>::=<deterministic_parameter>|<random_parameter>

To further explain the "primitive information" node defined in the material template, two examples are also provided here. In Figure 8, the "primitive information" node of the BCC lattice is given. In this case, the material is made of periodically distributed BCC unit cells. Thus, the unit cell of the BCC lattice material is defined as the only primitive under this node. The unit cell of BCC lattice can be further divided into 20 cylindrical struts. The shape of each strut is controlled by the corresponding implicit function. In the implicit function, deterministic parameter d is defined to control the shape of a strut. The value of this parameter is directly from the descriptor d defined in the descriptors list.

Another example is the short fiber-reinforced composite. Its "primitive information" node is shown in Figure 9. It only contains a single primitive – short fiber. Unlike the BCC lattice material discussed above, the short fibers of this material are stochastically distributed inside its matrix material. Thus, to describe the shape of short fibers, a single independent random parameter is defined in its implicit function. Particularly, parameter d represents the diameter of a fiber. The value of this random variable is controlled by the defined PDF under the node "independent random parameter 1". In its PDF, (σ_d, u_d) are two descriptors defined in the descriptors list. These two parameters can control the distribution of fiber diameter.

3. Examples

Based on the developed material template, the RVEs of two different types of materials discussed in the previous section have been reconstructed. In the following contents of this section, the relationship between material descriptors defined in the material template and its corresponding microstructures will be carefully discussed.

3.1 Short fiber-reinforced composite materials

Based on the material template described in Section 2, the RVEs ($5\ mm \times 5\ mm \times 5\ mm$) of short fiber reinforced composite have been reconstructed and shown in Figure 10. For the visualization purpose, only fibers are displayed in Figure 10, while matrix material is kept as transparent. To further illustrate how the values of material descriptors defined in the material template affect its microstructures, two material descriptors σ_θ and v_f are varied case by case, while other material descriptors are set as constants. The values of constant material descriptors are summarized in Table 1.

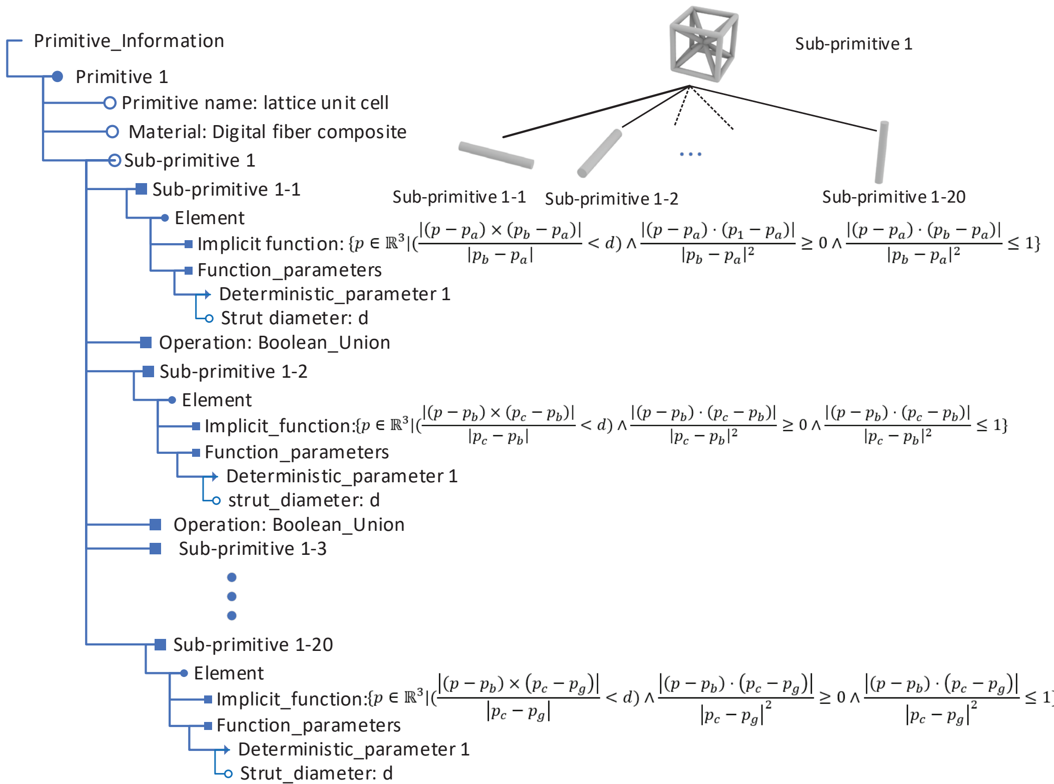


Figure 8 “Primitive Information” node for BCC lattice

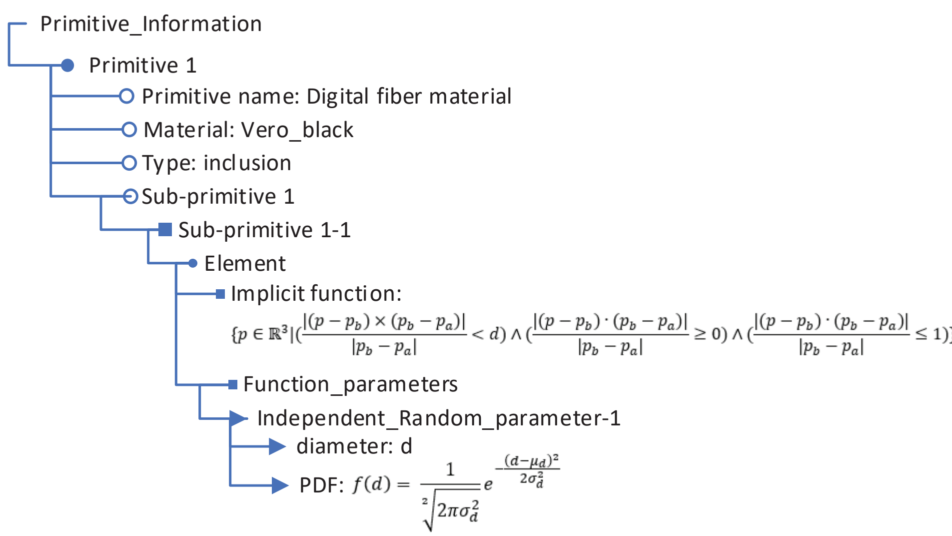


Figure 9 “Primitive Information” node for the fiber-reinforced composite

Table 1 The values of material descriptors for the RVEs of the short fiber reinforced material

μ_d	σ_d	μ_θ	μ_ϕ	σ_ϕ	μ_r	σ_r
0.2mm	0.02mm	$\frac{\pi}{2}$	0	$\frac{\pi}{20}$	1mm	0.05mm

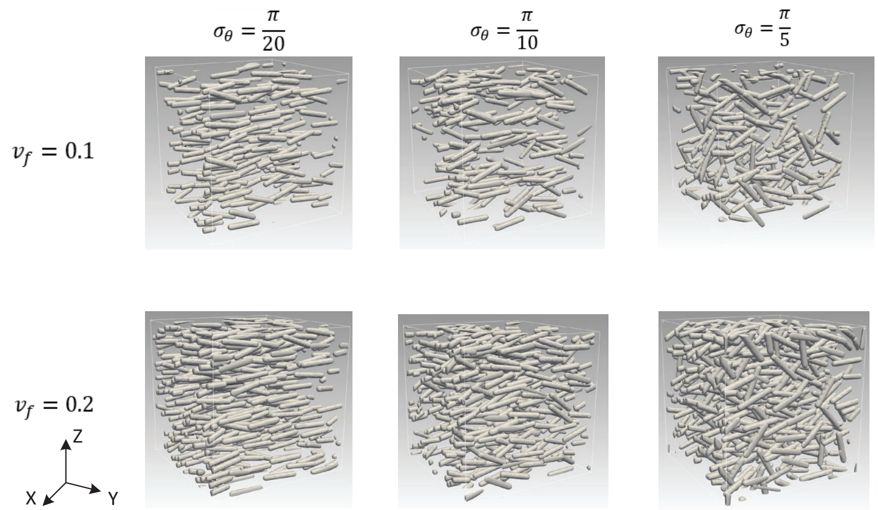


Figure 10 The RVEs of fiber-reinforced composite with different materials descriptor values

Figure 10 shows a clear trend that material descriptor v_f can accurately control the volume fraction of fibers. More fibers are included in the RVE when v_f increases. σ_θ is the descriptor that can be used to control the distribution of fiber's orientation angles. A decrease of σ_θ will make the fibers well aligned along a single direction.

3.2 BCC lattice material

In the second example, the RVEs of BCC lattice materials are reconstructed based on the developed material template and its associated material descriptors. In this example, both descriptor d and descriptor l_c are changed. The reconstructed RVEs of BCC lattice materials are shown in Figure 11. In this figure, each RVE contains 5 x 5 x 5 lattice unit cells. As it is shown in Figure 11, by changing the descriptor d, we can obtain the lattice with different strut diameters. By changing the descriptor l_c, RVE with different cells size can be generated. By controlling these two descriptors simultaneously, we can obtain lattice with different relative densities. It indicates that the material descriptors defined in the material template developed in this paper can also be converted to the conventional material descriptors used for lattice materials such as relative density or porosity.

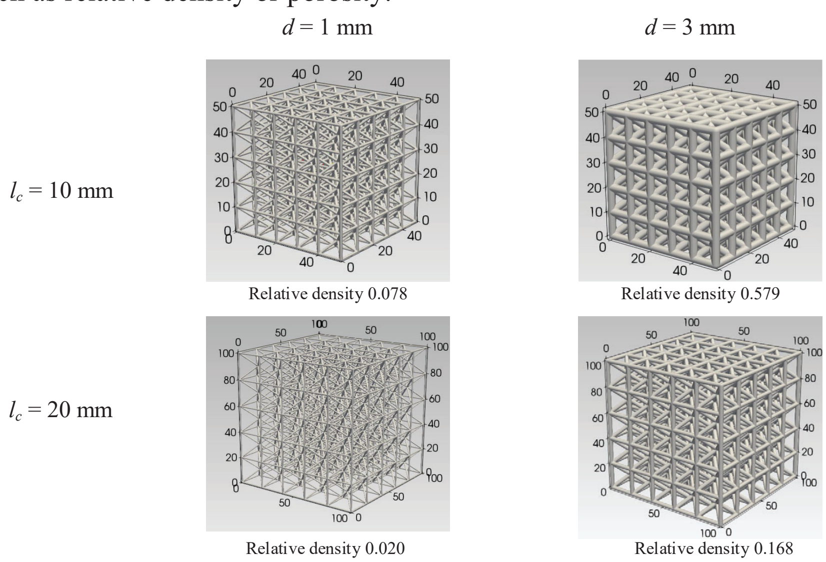


Figure 11 The RVEs of a BCC lattice material with different material descriptors

4. Summary and Future Research

In this paper, we developed a universal material template that can be used to quantitatively characterize the microstructure of different materials. In general, the developed template is organized in a hierarchical structure. The root node of the template contains four sub-nodes: “descriptors list”, “constituent materials”, “position information” and “primitive information”. The format of each sub-node has been given in this paper to help users to establish a standardized description of microstructures of materials. Two examples have been provided in this paper to help readers to understand the overall structure of the developed template. Also, these two examples prove that the developed method can be used to effectively describe the materials with both periodic microstructures and stochastic microstructures. Future work includes developing multiscale heterogeneous modeling method based on the developed material template in this paper. The developed method can describe both the material’s compositions and microstructures on multiple design scales. It can further enlarge the design freedom enabled by additive manufacturing and helps designers to improve the performance of the designed part by controlling the design parameters defined on multiple design scales.

Acknowledgment

The authors acknowledge support from the Digital Manufacturing and Design (DManD) research center, funded by the Singapore National Research Foundation, at the Singapore University of Technology and Design.

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