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Material-Unit Network for Multi-Material-Property and Multiscale Components

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Abstract. Additive Manufacturing (AM) increases much design freedom for designers to conceive parts with complex geometries and material information. However, the increased complexity makes it difficult to model heterogeneous objects defined on a multiple design scale. To solve this problem, an innovative modeling framework is proposed in this paper to enable the modeling of structures with multiscale complexities. Several examples are used to demonstrate the feasibility of applying the proposed method for representation of multi-material-property and multiscale components.

Keywords: Multi-Material-Property Component, Multiscale, Material-Unit Network, Additive Manufacturing.
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1 INTRODUCTION

Currently, additive manufacturing technologies have already been widely used to fabricate parts with complex geometries. Porous structures with multiscale complexities can be fabricated by AM process without support structures [29]. To take advantages of design freedom provided by AM, several design methods for additive manufacturing [18] has been developed. However, it should be noted that most existing design methods only focus on structure's geometry. Thus, most parts designed by existing DfAM (Design for AM) methods are made of single materials [25].

To further improve the performance of designed products, concurrent optimization methods [2,4] which can update the distribution of material microstructures and structure's macro geometry have been developed. Comparing to design optimization method focused on a single design scale, concurrent optimization methods can achieve better performance especially for design cases for multifunctional purposes. Even though, those concurrent optimization methods are promising in terms of their performance, none of the results of these optimization methods have been successfully fabricated by existing AM technologies. It is difficult to model the optimized results in existing commercial CAD software. The modeling techniques used in existing commercial CAD software only capable to deal with geometry with single material defined on a single design scale. To solve this problem, an innovative modeling framework is proposed in this paper to enable the modeling of structures with multiscale complexities.

In this paper, a novel material-unit network is proposed for representation of multi-material-property component for AM. The remainder of this paper is organized as follows: In Section 2, the related work is briefly reviewed in the literature. The definition of multi-material-property component is given in Section 3. Section 4 presents the detailed description of material-unit network. Based on the proposed material-unit network representation, several examples are offered in Section 5 to show the efficacity and flexibility of the proposed approach. Section 6 discusses the conclusions of this study and future work.

2 RELATED WORK

Many scholars have carried out an in-depth research on the representation of heterogeneous objects modeling. It mainly includes the decomposition-based representation, set based representation, topology hierarchy feature based representation and parameter control point representation. A brief review of the methods is provided here to clarify the difference and limitations of present works:

- Decomposition based representation: Based on the idea of space segmentation, the space body is divided into grid elements, such as voxel element and finite element meshes, and the decomposition representation method is proposed[9,10,17,27].The material information of the voxel element is stored in the voxel center point, which is suitable for the irregular distribution of the material. It not only supports the efficient query of the material composition, but also facilitates the realization of visualization. In addition, its three-dimensional array structure is also beneficial for parallel execution. However, the pitfall of the voxel model is also obvious. The accuracy of the method is directly related to the voxel's resolution. To get an accurate heterogeneous model, huge storage spaces are usually needed. Moreover, voxel methods are inexact in terms of the geometric and material accuracies. The material information of the finite element meshes model is stored in the grid node, and the material information of the non-grid node is saved by the interpolation function. Therefore, the representation is a more compact data structure, which solves the huge storage problem in voxel unit to a certain extent, and it can express more complex material distribution. However, there are also a few inherent limitations: Because of the interpolation mechanism, the material distribution of the non - vertex of the grid can't be accurately expressed and preserved. In the material interrogation, the boundary facet which has the minimum distance to the query point must be first identified. As the boundaries of the object has been discretized into many facets, searching the facet through all the boundary facets may be time consuming.
- Set based representation: Based on the r_m-set, level set and R function set respectively, the set-based representation is established and the Boolean set operation including material information is constructed. The multi-material objects with more complex geometry and material distribution are obtained [15,24,26].The model represents material domain boundaries with B-rep. Each material domain contains only one material, which is well suited to represent composite objects that have significant demarcation between materials. However, this representation is not suitable for multi-material mixing objects.
- Topology hierarchy feature based representation: Based on the distances of points to reference features distributed to known or predefined materials, a topological hierarchical feature is established [7,8,14,16,19,22,23]. The representation can realize different material gradients through the material distribution function, and realize the multi-material object modeling that meets the design intent. The material distribution is

invariant under some transformations, such as rotation or translation. Due to the effective evaluation of point-to-feature distances, the representation supports efficient query of material composition. Moreover, the user can select the reference features and material distribution function through the predefined function library, and can intuitively and flexibly complete the interaction modeling of multi-material objects.

- Parameter control point based representation: The material information is stored in the control points of Bezier, B spline, NURBS, parameter curve, surface and body, and the representation of parameter control point is obtained [3,20,21,30].Control point based models have some appealing properties. They are compact in both geometry and material representations. Given the parametric coordinate (u, v, w), the material composition of a point can be also efficiently interrogated. In addition, this representation method can effectively represent complex (2D or 3D dependent) material distributions. Local modifications on both geometries and material definitions are also straightforward. The drawback of this method is that it relies heavily on spatial parameterizations and for arbitrary 3D objects such parameterizations remain a rather non-trivial task.

However, the above research approaches only focus on continuous distribution of material composition modeled parametrically by volume fraction, which is applied to solid part model on macro scale instead of material microstructure on lower scale. It is inaccurate because microstructures with the same material volume fraction may have different topological geometry and properties. The appropriate representation is that material microstructure forms the basis for material volume fraction. For instance, nanotechnology enables engineers to create or modify details of atoms at nanoscales so as to realize more desirable material properties. As this technology becomes more pervasive, it is foreseen that some materials modeling modules will be embedded in future CAD systems so that the geometry and materials of a product can be designed concurrently [12].

Rosen et al. firstly proposed a new multiscale geometric and materials modeling method that uses a surfacelet-based implicit representation to efficiently capture internal and boundary information of materials. It serves as the foundation for modeling structure-property relationships for materials design [11,13,28]. Gomes et al. present that at the highest level of abstraction, the object morphology is hierarchically defined by means of a graph, called Feature Interaction Graph (FIG), whose nodes represent form features and whose arcs represent their interaction relationships[5,6]. As a result, the research findings above provide guidance and new ideas for follow-up research.

3 MULTI-MATERIAL-PROPERTY COMPONENTS

Figure 1 represents the bone's multi-scale configuration from the five scales of nanoscale, sub-microscale, microscale, mesoscale and microscale [1]. It can be seen that the whole bone has different constituent elements at different scales, and each element corresponds to different geometry, material and property information.

With the further development of AM technology, it can be inferred that this kind of configuration shown in Figure 1 will be the main component of future products, and also the common object of future product manufacturing.

In this paper, an independent shape or structure with the following features in space is called a **Multi-material-property Component**:

① Limited size;

② The shape and structure are composed of a set of geometric elements such as points, curves, surfaces and/or solids;

③ Within each geometric element (including a point), one or more materials are distributed in a certain way.

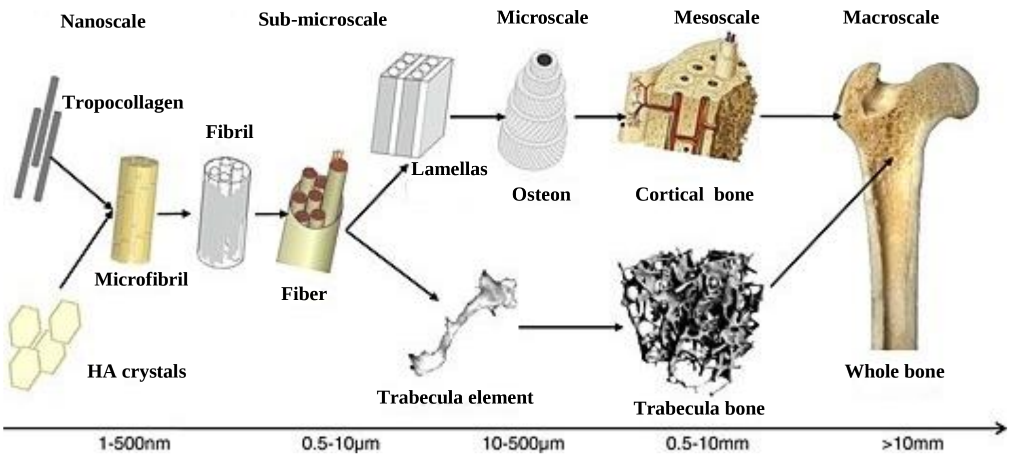

Figure 1: Multi-scale configuration for bone.

It can be seen from the above definition that the **multi-material-property component** studied in this paper not only retains the "limited size" of the traditional component structure, but also adds low-dimensional geometric elements such as points, curves and surfaces to the macro-structure composition, which is further speculated and expanded based on AM. On the microscopic aspect, the introduction of multi-material-property distribution has created conditions for further improving the performance of product components that are traditionally distributed only with a single variety of materials.

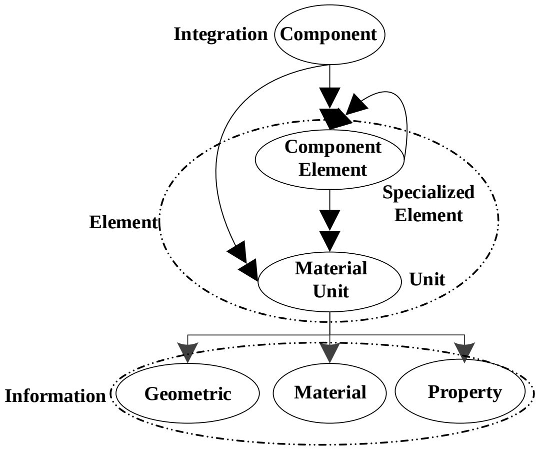

Figure 2: Multi-material-property configuration.

Without considering the differences in the definition scales of these structures and shapes, and the components are analyzed, recognized and defined uniformly from three levels: integration, element and information (Figure 2). Among which, the element layer is subdivided into two levels, namely, the component element and material unit, which are defined as follows:

①**Component Element**. A specialized element is defined according to the structure and shape features of a certain type of component, and only represents the composition of the component.

② **Material Unit**. A continuous region with the same material and pattern of property distribution is defined as a material unit, which is the most basic unit of multi-material-property component.

Figure 3 shows an explanation of the multi-material-property and multiscale configuration of bone. At nanoscale the microfibril is composed of two kinds of component elements, the skin and core of microfibril. The corresponding material units are Cylinder 1 and red Cylinder 2, respectively. Cylinder 1 is made up of HA crystals and Cylinder 2 is made up of tropocollagen, owning different properties.

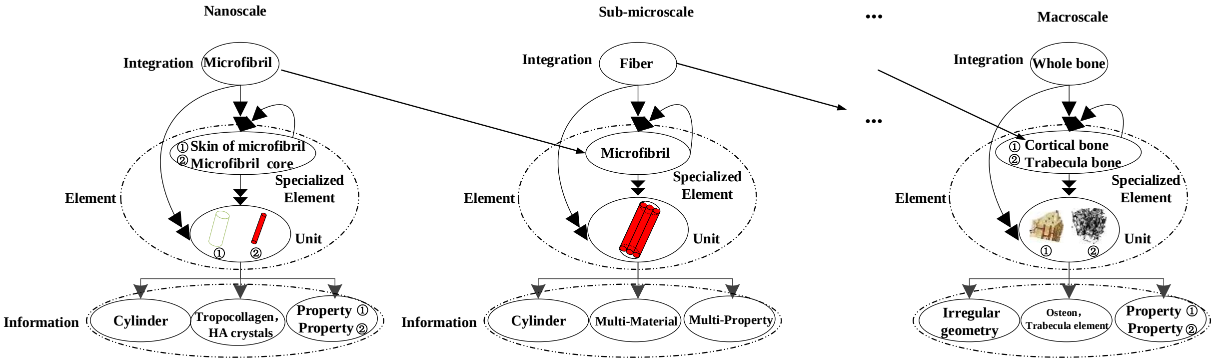

Figure 3: Explanation of multi-material-property and multiscale configuration of bone.

4 MATERIAL-UNIT NETWORK

The results of all the multi-material-property operations of the above-mentioned component models are a group of material units which are adjacent to each other. We use graph to define and represent the operation result, which is called the material-unit network. Since the material unit and their adjacency relationships have certain specific properties and types, it is necessary to expand the concept of "graph" in mathematics before defining and establishing the material-unit network, and the extended graph is called " Extended Network ".

4.1 Extended Network

The definition of edge $e(e \in E)$ in graph $G = (V, E)$ are expanded as follows

$$e = \bar{e} \mid \vec{e} \tag{4.1}$$

where $\bar{e}$ is an undirected edge that represents the same set of unordered relationships among vertices and is denoted as

$$\bar{e} = < v_i \mid v_i \in V, i = 1,2,\ldots,n_{ev} > \tag{4.2}$$

$\vec{e}$ is a directed edge that defines an ordered relationship between vertex v_1 and v_2, which is denoted as

$$\vec{e} = (v_1, v_2 \mid v_1, v_2 \in V) \tag{4.3}$$

where vertices v_1 and v_2 are called start and end vertex of $\vec{e}$.

The above definition of G is called the Extended Network. The intuitive representation of edges in extended network is shown in Figure 4.

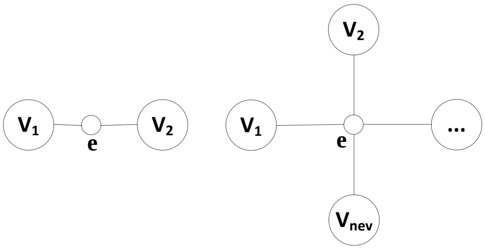

Figure 4: Edges of extended network: (a) directed edge, and (b) undirected edge.

Let e be an edge of $G=(V,E)$, i.e., $e \in E$, n_{ev} be the number of vertices on e, then n_{ev} is called the edge degree of e and denoted as $n_{ev}=d(e)$, and we specify $n_{ev} \geq 2$.

Property:

① Let $\bar{e}$ be an undirected edge of Extended Network $G=(V,E)$, then $d(\bar{e}) \geq 2$.

② Let $\vec{e}$ be an directed edge of Extended Network $G=(V,E)$, then $d(\vec{e}) \equiv 2$.

4.2 Material-Unit Network

The extended network is used to define and represent a component C, namely:

$$C=(U,R) \tag{4.4}$$

where vertex set U is the set of all component element and material unit (hereinafter collectively referred to as material unit) $u_i(i=1,2,\ldots,m)$, namely:

$$U=\{u_1,u_2,\ldots,u_m) \tag{4.5}$$

Edge set R is the set of all relationships $r_j(j=1,2,\ldots,n)$ between $u_i(i=1,2,\ldots,m)$, namely:

$$R=\{r_1,r_2,\ldots,r_n) \tag{4.6}$$

The structure defined in Equation (4.4) is called the **Material-Unit Network** of a component. The intuitive definition of relationship r is shown in Figure 5, where 0 and 1 on the connecting line respectively define the correlation between material unit and relationships, if there is no special annotation, 1 indicates correlation.

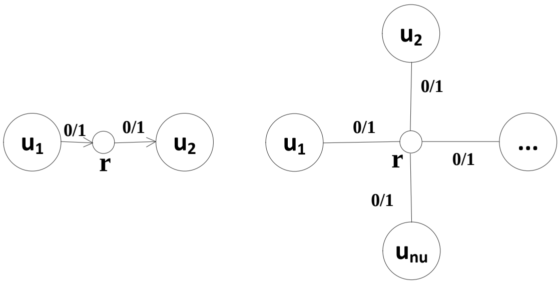

Figure 5: Relationship of material unit: (a) directed edge, and (b) undirected edge.

Actually, let material-unit network at lower scale be a material unit at upper scale, the material-unit network can be expanded to multiscale material-unit network and has the ability to express multiscale component (Figure 6).

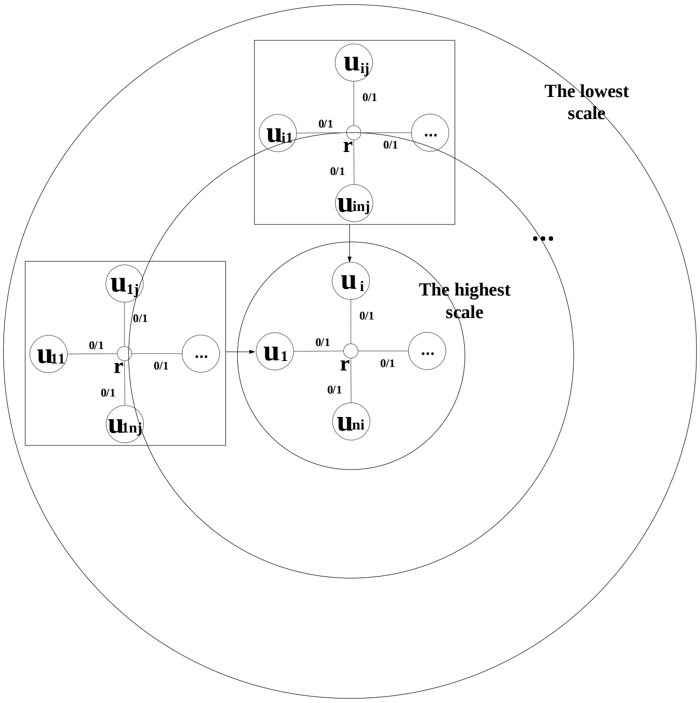

Figure 6: Multiscale material-unit network.

4.2.1 Relationships between material units

Let r be any one of relationships of R, i.e., $r \in R$, then r can be represented as

$$r = < u_i(g_i) \mid u_i \in U, i = 1,2,\ldots,n_u > \tag{4.7}$$

which means that there is a relationship between the boundary element g_i in $u_i (i = 1,2,\ldots,n_u)$, $n_u = d(r)$.

4.2.2 Associated unit

We call $u_i (i = 1,2,\ldots,n_u)$ inEquation（4.7） the associated material unit, or **Associated Unit** for short, and g_i is called the associated boundary element, or **Associated Element** for short. The set of all the associated material units of r is called the associated unit set, denoted by $U(r)$, which is:

$$U(r) = \{u_i \mid u_i \in U, i = 1,2,\ldots,n_u\} \tag{4.8}$$

The set of all the associated elements is denoted as $B(r)$, which is:

$$B(r) = \{g_i \mid u_i(g_i), u_i \in U, i = 1,2,\ldots,n_u\} \tag{4.9}$$

If both b and g are boundary elements of material unit u, and b is the composition of g or equals g, we unify the representations as $b \in g$.

4.2.3 Overlapping relationship

Let $r_1 =< u_1^i(g_1^i) \mid i = 1,2,...,n_1 >$ and $r_2 =< u_2^i(g_2^i) \mid i = 1,2,...,n_2 >$ be two relationships, if the following conditions are both met:

a. $d(r_1) = d(r_2)$, i.e., $n_1 = n_2$;

b. For any boundary element g_2 of $B(r_2)$, $\exists g_1 : g_1 \in B(r_1) \wedge g_2 \in g_1$, i.e., g_2 is also a boundary element of $B(r_1)$ or the composition of one of the boundary elements. Then r_2 is called the Overlapping Relationship of r_1.

Axiom: There is no overlapping relationship in a material-unit network.

4.2.4 Cluster of relationships between material units

In a material-unit network, set u_1 and u_2 be two material units, then all the relations between them are recorded as $R(u_1, u_2)$, namely:

$$R(u_1,u_2) = \{r \mid u_1 \in U(r) \wedge u_2 \in U(r)\} \tag{4.10}$$

That is to say, $R(u_1,u_2)$ is a set of all relations r between associated unit u_1 and u_2, $R(u_1,u_2)$ is called the cluster of relationships between material units.

5 EXAMPLE

Four examples of Material-Unit Network are shown as follows:

Example 1: As shown in the Figure 7, all relationships between u_1 and u_2 are:

1. $r_1 =< u_1(e_1), u_2(e_2) >$
2. $r_2 =< u_1(v_1), u_2(e_2) >$
3. $r_3 =< u_1(e_1), u_2(v_2) >$

Obviously, r_2 and r_3 are Overlapping relationship of r_1.

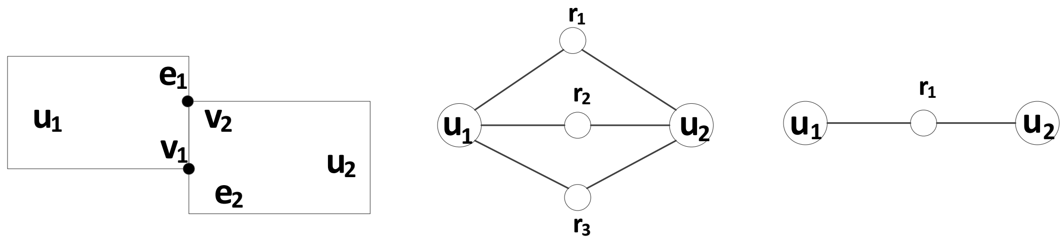

Figure 7: Example 1: (a) component, (b) relationships of material unit, and (c) material-unit network.

Example 2: As shown in the Figure 8, all relationships among u_1, u_2 and u_3 are:

1. $r_1 =< u_1(e_1), u_2(e_{21}) >$
2. $r_2 =< u_1(e_1), u_3(e_{31}) >$

3. $r_3 =< u_2(e_{22}), u_3(e_{32}) >$
4. $r_4 =< u_1(e_1), u_2(v_{22}), u_3(v_{31}) >$
5. $r_5 =< u_1(e_1), u_2(v_{21}) >$
6. $r_6 =< u_1(e_1), u_3(v_{32}) >$
7. $r_7 =< u_2(v_{23}), u_3(v_{33}) >$

Obviously, r_5, r_6 and r_7 are overlapping relationships of r_1, r_2 and r_3 in turn.

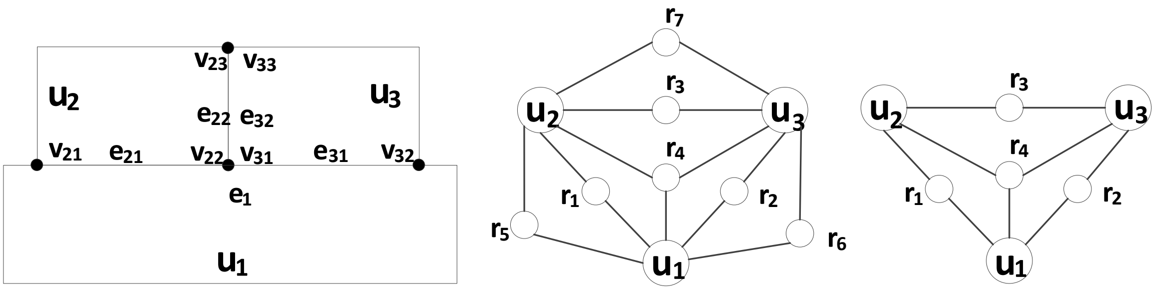

Figure 8: Example 2: (a) component, (b) relationships of material unit, and (c) material-unit network.

Example 3: As shown in the Figure 9, the relationships among u_1, u_2, u_3 and u_4 in the material-unit network are:

1. $r_1 =< u_1(e_{11}), u_2(e_{21}) >$
2. $r_2 =< u_2(e_{22}), u_3(e_{31}) >$
3. $r_3 =< u_3(e_{32}), u_4(e_{42}) >$
4. $r_4 =< u_4(e_{41}), u_1(e_{12}) >$
5. $r_5 =< u_1(v_{11}), u_2(v_{21}), u_3(v_{31}), u_4(v_{41}) >$

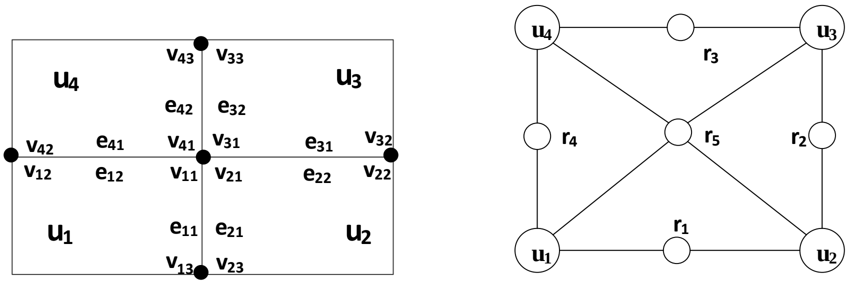

Figure 9: Example 3: (a) component, and (b) material-unit network.

Example 4: As shown in the Figure 10, the relationships among u_1, u_2 and u_3 in the material-unit network are:

1. $r_1 =< u_1(e_1), u_2(e_{21}) >$
2. $r_2 =< u_2(e_{22}), u_3(e_3) >$
3. $r_3 =< u_1(v_{11}), u_2(v_{21}), u_3(v_{31}) >$
4. $r_4 =< u_1(v_{12}), u_2(v_{22}), u_3(v_{32}) >$

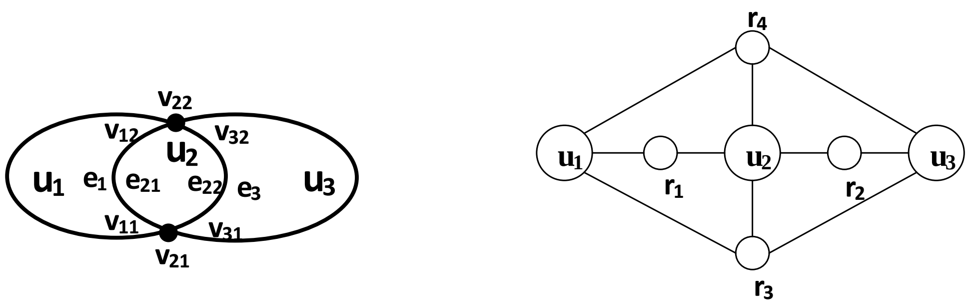

Figure 10: Example 4: (a) component, and (b) material-unit network.

Example 5: A microfibril at nanoscale from Figure 1 is used to illustrate material-unit network shown in Figure 11, u_1 represents skin of microfibril and consists of Side S_{11}. u_2,u_3 is tropocollagen that makes up core of microfibril, which consist of Side S_{21}, Plane S_{22},S_{23} and Side S_{31}, Plane S_{32},S_{33} respectively. The relationships among u_1,u_2 and u_3 in the material-unit network are:

1. $r_1 =< u_1(s_{11}), u_2(s_{21}) >$
2. $r_2 =< u_2(s_{21}), u_3(s_{31}) >$
3. $r_3 =< u_1(s_{11}), u_2(s_{22}) >$
4. $r_4 =< u_1(s_{11}), u_2(s_{23}) >$
5. $r_5 =< u_2(s_{22}), u_3(s_{32}) >$
6. $r_6 =< u_2(s_{23}), u_3(s_{33}) >$

Obviously, r_3,r_4 and r_5,r_6 are Overlapping relationships of r_1 and r_2 in turn.

Based on the material-unit network for microfibril at nanoscale, the multiscale material-unit network for the multi-material-property and multiscale configuration of bone from Figure 3 can be expressed in Figure 12.

Around the above mentioned material-unit network, the common object design pattern is used to define each object class, including refining and defining data members such as geometry, material, property, and related data processing functions of each object class, and on that basis, we establish the relationship between object classes, as shown in Figure 13 "vertex" refers to the vertex of "graph", which is the abstraction of "material unit" and "component". This pattern is based on the "composite" object pattern.

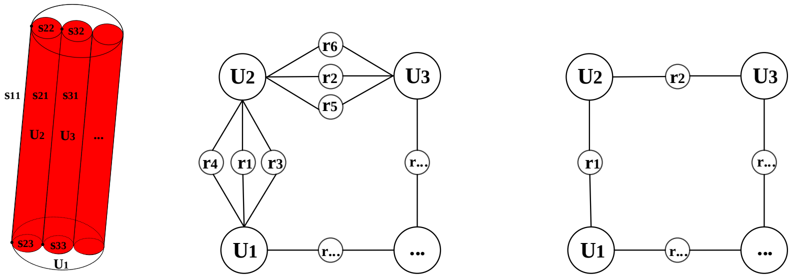

Figure 11: Example: (a) microfibril component, (b) relationships of material unit, and (c) material-unit network.

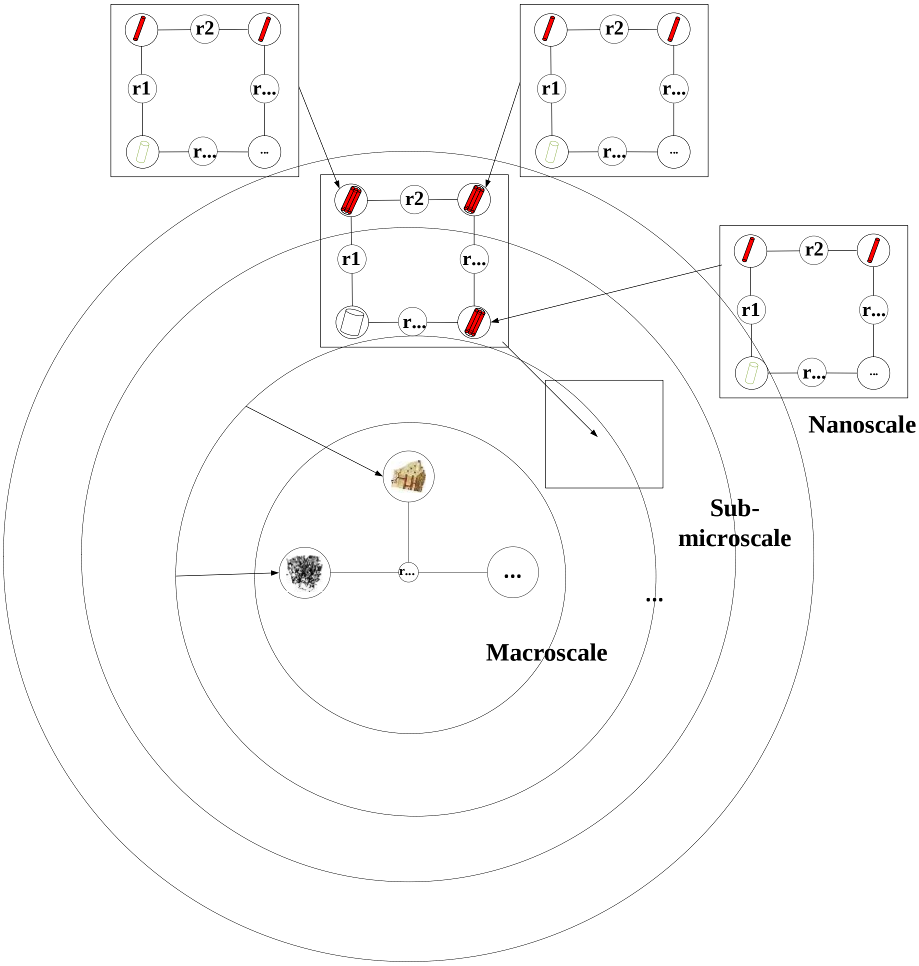

Figure 12: Multiscale material-unit network for multiscale configuration of bone.

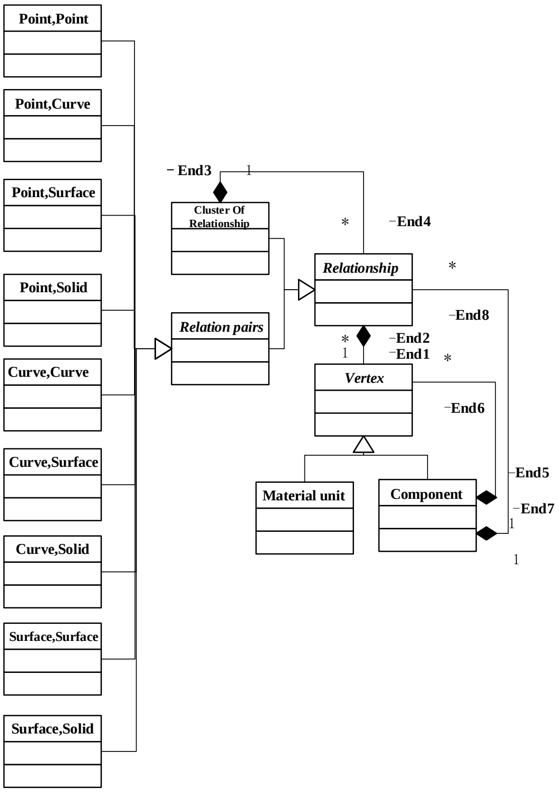

Figure 13: Material-unit network object pattern.

6 CONCLUSION

The innovative work of this paper is mainly as follows:

1. In this paper, the concept of multi-material-property and multiscale component for added material manufacturing is proposed, and the component is defined uniformly from three levels: integration, element and information

2. A data structure based on extended graph is proposed to define and represent the material units and their relationships. One of the "vertices" defines only the material unit and its spatial location data and does not contain specific information such as geometry, materials and properties of the material unit. Therefore, the sharing of the same material unit data can be realized, and the scale of model data is significantly reduced.

3. Based on the developed material-unit network, a set of operations will be defined to enable the generation and modification of multiscale objects. These operations mainly include Boolean operation such as difference, union, intersection. Comparing to existing boolean operations algorithm, the developed operations and their related algorithms involve the calculation on both materials and geometries. Thus, more research needs to be done to investigate how to apply these operation algorithms on both materials and geometries.

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