Solid Modeling of Nanoscale Artifacts

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ABSTRACT

Solid modeling involves creation and manipulation of complete and unambiguous mathematical representations of 3-D objects. The purpose of such a representation is to provide tools for visualization, calculation of geometric properties and realization by design and manufacturing processes. Existing methods of solid modeling namely constructive solid geometry (CSG), boundary representation (B-rep) and decomposition methods are found to be inadequate for representing nanoscale artifacts as they do not account for arrangement of atoms and molecules in the form of lattice structures, lattice planes and lattice constants. The proposed work is a step in the direction of bridging this gap. The paper presents a new solid modeling scheme for representing nanoscale artifacts. The applicability and effectiveness of the new representation is demonstrated by taking many examples including devices such as nanotubes.

Keywords: solid modeling, crystalline structure, constructive solid geometry, boundary representation, spatial enumeration

1 INTRODUCTION

Solid modeling involves the creation and manipulation of complete, unambiguous mathematical representations of 3-D objects. The purpose of such a representation is to provide tools for visualization, graphical user interaction and calculation of geometric properties needed at various stages of product life cycle. Geometric model of an object also forms a basis for integrating various life cycle activities, particularly product design and manufacturing. Existing methods of solid modeling can be classified into one of three major categories: constructive solid geometry (CSG), boundary representation (B-rep) and decomposition methods [1].

Constructive solid geometry (CSG) is a solid modeling method that combines simple solid primitives to build more complex models using Boolean operators: *union, difference* and *intersection* [2]. The resulting model is a procedural model stored in the mathematical form of a binary tree where leaf nodes are solid primitives, correctly sized and positioned, and each branch node is a Boolean operator. In a CSG representation, geometry and topology of an object is stored implicitly. This representation is not convenient to use for nanoscale artifacts, as it would be impractical to build and model an artifact as a Boolean combination of individual atoms / molecules.

In a B-rep scheme, [3] the solid objects are represented as unions of their boundaries or enclosing surfaces. The enclosing surfaces can include planar polygons, quadrics and free-form surface patches. In this scheme topological and geometric information are explicitly defined. Topological information provides the relationships among vertices, edges/curves and faces/patches. In addition to connectivity, topological information also includes orientation of edges and faces etc. Geometric information usually consists of equations of the edges/curves and faces/patches. B-Rep too has limitations in representation of nanoscale artifacts as it is difficult to identify a group of atoms / molecules that can define unique boundary surface of an object. Moreover, any such representation will have a few hundreds and thousands of boundary atoms / molecules to represent an object.

In decomposition methods, a solid is decomposed into a collection of adjoining, non-intersecting solid primitives. Depending on the shape and parameterization of primitives, decomposition schemes of solid modeling primarily have three general forms: spatial enumeration, cell decomposition and Octree encoding [4]. Spatial enumeration is a direct approach to solid modeling representation in which a solid is modeled as a collection of identical volume cells. Correct object representations are easy to maintain but difficult to create due to the simplistic structure. Cell decomposition is a generalization of spatial enumeration in which objects are represented as a collection of simple primitives, which are not necessarily required to have the same size or shape. A special case of cell decomposition/spatial enumeration modeling is *voxel based modeling* in which object is modeled as a collection of cubical cells of same size which are located in a fixed grid in a 3D discrete space.

The octree encoding [5, 6] is similar to both spatial enumeration and cell decomposition in that, objects are represented as a collection of fundamental primitive solids or cells. However, the representation is made more efficient by organizing the cells in an eight-array tree. Cells that are partially full are further subdivided into cells. However the storage required increases exponentially as the tree depths increase.

The above discussed decomposition methods of solid representation are used to model solid objects whose dimensions can go as small as a few micrometers [7]. The same representations have limitations in modeling nanoscale artifacts as the cell and grid sizes reach dimensions comparable to inter-atomic distances. However, among the three major solid modeling schemes discussed above, the decomposition methods are closest in terms of representing arrangement of individual atoms and molecules with which any 3D object is made of. It was felt decomposition methods with some modifications could be used as potential tools for modeling nanoscale artifacts.

2. GEOMETRY OF CRYSTALLINE SOLIDS

Solids can be broadly classified as crystalline and amorphous solids. In a crystalline solid, the arrangement of atoms is in periodically repeating fashion, whereas no such regularity of arrangement is found in amorphous solids. Such an arrangement of atoms in a crystalline solid is referred as space lattice. The space lattice can be defined by referring to a unit cell. The unit cell is defined as the smallest unit which, when repeated in space indefinitely will generate a space lattice. Thus the geometry of crystalline solids can be modeled as an array of unit cells in three dimensions in which every point has surroundings identical to that of every other point in the array. There exist 14 different types of space lattices, known as Bravais Lattices, which belong to seven different crystal systems. For example one of the seven crystal systems is cubic crystal system is defined by three mutually perpendicular translation vectors, which are equal in magnitude. The magnitude of this vector is fixed for a given material and can be defined in terms of lattice constant For example the lattice constant for Aluminum is 0.321 nm (nano meters), and that of Iron is 0.287 nm. The three space lattices in the cubic crystal system namely Simple Cubic (SC), Body Centered Cubic (BCC) and Face Centered Cubic (FCC) are shown in the Table 1.

The crystalline solid looks different when cut at different orientations. System of Miller indices is the universally accepted system of indices that has been developed to describe the orientation of crystallographic planes and crystal faces relative to crystallographic axes. Miller Indices are a symbolic vector representation for the orientation of an atomic plane in a crystal lattice and are defined as the reciprocals of the fractional intercepts, which the plane makes with the crystallographic axes (**x, y** and **z)**. Miller indices are represented by a set of 3 integer numbers <hkl>. For example if **x, y** and **z** intercepts of a plan are 2, 1 and 3 respectively, the Miller indices are <362> obtained by multiplying the reciprocal of **x, y** and **z** intercept values (½, 1 and ⅓) to convert them into integers. Table 2 shows typical planes and the corresponding Miller indices for cubic crystal system.

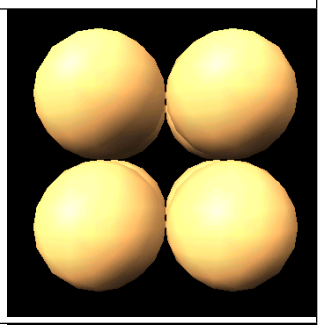
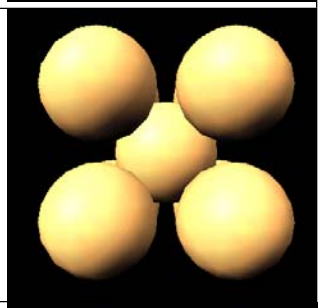
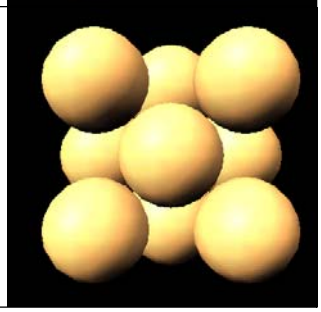
Lattice Structure	Effective number of atoms per unit cell	Figure
Simple Cubic (SC) Atoms at Eight corners of unit cell	1	
Body Centered Cubic (BCC) Atoms at Eight corners and at the center of unit cell	2	
Face Centered Cubic (FCC) Atoms at Eight corners and at center of six faces of unit cell	4	

Table 1: Cubic Crystal System

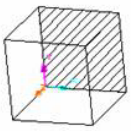
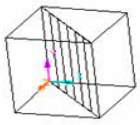
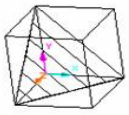
Miller Indices	<100>	<110>	<111>
Illustration			

Table 2. Miller Indices for Cubic Crystal System

3. MODELING OF NANOSCALE OBJECTS

The new solid modeling representation proposed for nanoscale artifacts is discussed in this section. The proposed representation has some similarities with decomposition models discussed earlier. In the present scheme a solid object is represented as a number of

spherical primitives. These spheres are located in a grid like structure defined by one of the 14 Bravais lattice structures. Center of sphere corresponds with grid point and the radius of the sphere depends on the lattice constant. This type of model can be considered as a special case of decomposition scheme, with primitive as an atom with voids between it and surrounding atoms.

Every lattice structure has a template with fixed number of cells and their relative arrangement which when extended in lattice directions as an array, gives bulk of solid which we call as an extended structure. For example a 3D object in a cubic crystal structure can be represented as a three-dimensional array, the three directions of the array correspond to three crystallographic directions. Table 3 shows an extended structure for three different types of lattice structures of cubic system.

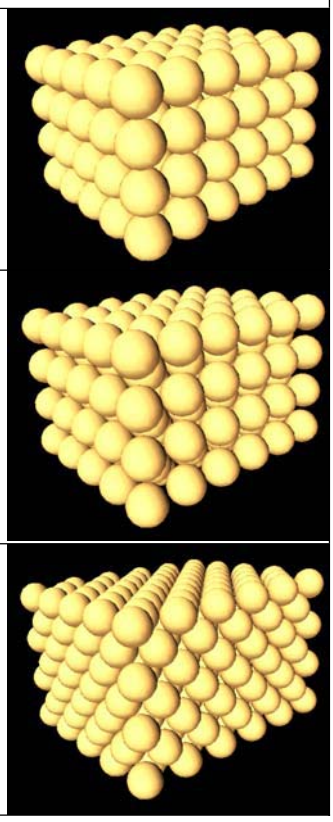
Number of cells in template	Lattice Type	Illustration
1	Simple Cubic (SC)	
2	Body Center -ed Cubic (BCC)	
4	Face Center -ed Cubic (FCC)	

Table 3. Extended structures of Cubic Crystal System

In order to construct solid model an object in the present scheme, first a boundary representation of the same is obtained. Next the size of array of an extended structure is chosen such that the object to be represented can be made to completely lie inside the structure. All the grid positions, which are contained in the object being represented, are binary coded 1 or else 0.

The generic representation of a solid in the present scheme has following format:

< t, a, **l** >
< Δ l_i * c binary data>

Where *t* corresponds to type of lattice structure, *a* corresponds to lattice constant, **l** is vector whose elements represent size of array along different crystallographic directions and *c* correspond to number of unit cells in template corresponding to lattice structure *t*. Figure 3 shows views of a 3D object in B-Rep and proposed scheme.

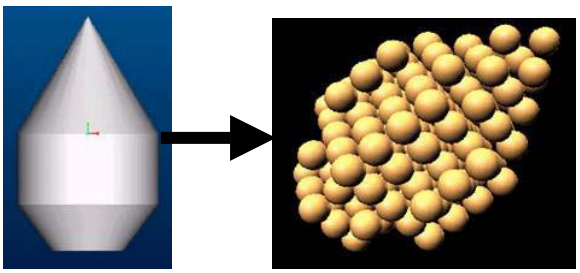


Figure 3. B-Rep and proposed model for a 3D object

Orientation of the object with respect to crystallographic direction is important parameter in the present system of modeling. In other words different orientations of the object with respect to given extended structure will yield different representations for the same object. This is true with other decomposition models such as octree encoding or voxel based modeling. Among the infinite orientations possible for the object with respect to crystallographic directions, some of the orientations have special significance from manufacturing point of view. Here the orientation of the object or object plane is be represented using a vector as an input. Such a representation has direct relation with Miller indices for crystal planes discussed earlier.

In the present work only a few of the fourteen Bravais lattice structures are discussed here. However extension of concept to other lattice structures is non-trivial.

4. RESULTS & CONCLUSIONS

The proposed scheme of solid modeling is used to construct and model many nanoscale artifacts. Tables 4 and 5 show results of modeling and visualization for two typical nanoscale artifacts, a stepped hollow shaft and a bracket. In the two cases the results of visualization are shown for same size of artifact but for different lattice structures or for different orientations. Solid modeling scheme discussed in the present work can be used for visualization of nanoscale artifacts and manipulation of the same leading to designs with preferred atomic terraces and orientations. Secondly it can be used for manufacturing of nanoscale artifacts, which

require preferred atomic planes for atomic level manipulations as it is done using STM probes [8].

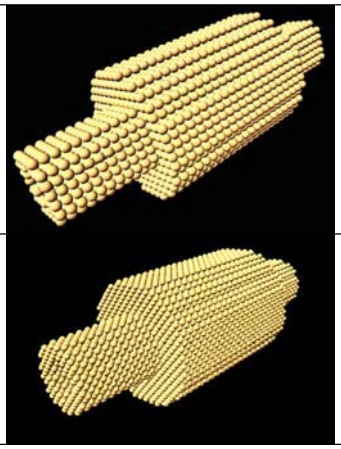
Lattice & Orientation	Illustration
Simple Cubic <100>	
Face centered Cubic <100>	

Table 4. Solid model of a Stepped Hollow Shaft

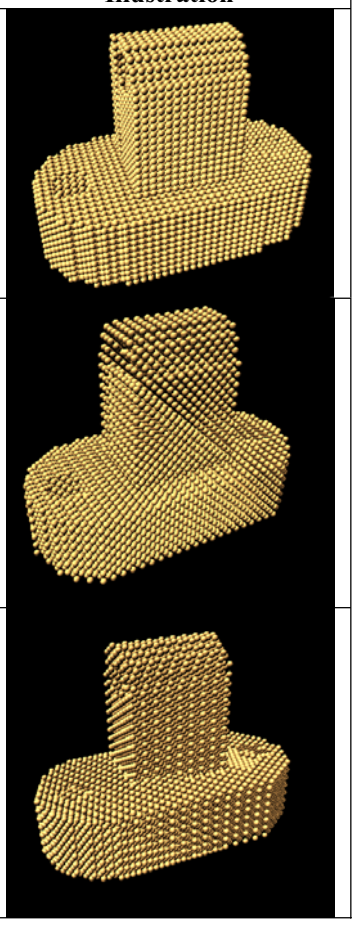
Lattice & Orientation	Illustration
Body Centered Cubic <100>	
Body Centered Cubic <110>	
Body Centered Cubic <111>	

Table 5. Solid model of a Bracket

In our present work modeling of only crystalline solids with lattice structures belonging to cubic system are dealt in detail. The model can be generalized for other lattice structures. Fig. 4 show a nanotube modeled using present scheme, which has hexagonal structure.

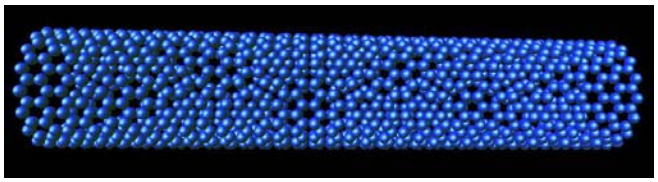


Figure 4. B-Rep and proposed model for a nanotube

A different approach is needed when modeling those objects, which consist of molecules and bonds in stead of objects made of single type of atoms. The real life artifacts are more complex in terms of geometry having crystal defects, dislocations and grain boundaries. We are presently extending our work along these lines and results if which will be communicated through another paper.

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