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# Periodic surface modeling for computer aided nano design

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#### Abstract

Current solid and surface modeling methods based on Euclidean geometry in traditional computer aided design are not efficient in constructing a large number of atoms and particles. In this paper, we propose a periodic surface model for computer aided nano design such that geometry of atoms and molecules can be constructed parametrically. At the molecular scale, periodicity of the model allows thousands of particles to be built efficiently. At the meso scale, inherent porosity of the model represents natural morphology of polymer and macromolecule. Surface and volume operations are defined to support crystal and molecular model creation with loci and foci periodic surfaces. The ultimate goal is to enable computer assisted material and system design at atomic, molecular, and meso scales. (© 2006 Elsevier Ltd. All rights reserved.

Keywords: Periodic surface; Minimal surface; Hyperbolic geometry; Computer aided nano design

#### 1. Introduction

To accelerate the development of nanotechnology, computer aided design tools are critical to solve the "lack of design" issue, which is that no extensive and systematic design of nano systems is available, compared to other traditional engineering domains such as mechanical mechanisms and electronic circuits. Computer aided nano design (CAND) is to enable engineering design, traditionally at macro scales, to be extended to nano scales. CAND helps to set functional objectives, construct models, simulate and optimize design, and guide laboratory efforts at physical property implementation.

Existing atomic and molecular simulation methods such as *ab initio*, density function theory, molecular dynamics, empirical force field, and Monte Carlo and related tools enable scientists to visualize molecular structure and behavior, calculate properties such as electrical conductivity, elasticity, and thermodynamics, as well as to simulate reactions between molecules. This simulation-based approach saves time and resources when conducting real experiments to study physical properties and interactions of molecules, in areas such as drug and material design. Material properties can solely be calculated, and the results become the input of bulk-scale finite element analysis. Nevertheless, in current simulation systems, atomic and molecular models can only be built by specifying geometric coordinates and bond connectivity explicitly. Lack of efficient and parametric compound constructing methods for atoms and molecules becomes the bottleneck of CAND. A good initial geometry is required to find an optimal molecular configuration in simulation. Providing nano engineers and scientists effective and easy-to-use tools to create a geometry conformation that is reasonably close to the true minimum energy is highly desirable. This is to save simulation time and lessen the risk of being trapped at local minima.

Furthermore, scalability of models should be considered. It is realized that there is a need of multi-scale computational models to address problems with different size and time scales during engineering design. Traditional geometric modeling methods do not consider multiple scales. How to build geometric modeling bridges in quantum, molecular, meso, and bulk scales with computational efficiency consideration is challenging.

In this paper, we propose a new surface modeling scheme to support multi-scale modeling and simulation. This surface based approach is to renovate existing boundary based model creation methods for atoms, molecules, and macromolecules, which create geometric models directly in Euclidean space. The proposed periodic surface model will allow rapid model construction and packing with thousands of elements

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in different compounds, which is time-consuming, if not impossible, with today's modeling approaches.

In the rest of the paper, Section 2 gives a brief overview of existing geometric modeling approaches in different scales, as well as minimal surfaces found in atomistic, molecular, and meso scales. Section 3 presents the proposed periodic surface model, which not only approximates minimal surfaces well but also represents various Euclidean and hyperbolic geometries. Associated surface and volume operations are defined. Section 4 describes model construction based on symmetric tiling and mapping methods of loci surfaces. Section 5 shows model creation based on foci surfaces, followed by discussions of implementation and future extensions in Section 6.

#### 2. Background

#### 2.1. 3D Geometric modeling methods

At the bulk scale, commonly used geometric modeling methods include boundary representation and constructive solid geometry for solid modeling, Hermite, Bézier, Bspline, T-spline and other polynomial functions for freeform surfaces, as well as convolution surface and R-function for implicit surface and volume respectively. Other modeling methods include wireframe, volume-based, point-based, and line geometry. At the meso scale, volume interfaces are usually approximated numerically such as isosurfaces. At the molecular scale, atoms and particles are represented by geometry (coordinates of positions in Euclidean space) and topology (connection between atoms). Traditional visualization methods for molecules include space-filled, wireframe, stick, ball and stick, and ribbon models.

To reduce graphics processing time, there has been some research on molecular surface modeling [1]. Lee and Richards [2] first introduced a solvent-accessible surface, the locus of a probe rolling over a Van der Waals surface, to represent the boundary of molecules. Connolly [3] presented an analytical method to calculate the surface. Recently, Bajaj et al. [4,5] represent a solvent accessible surface by NURBS (non-uniform rational B-spline). Carson [6] represents molecular surfaces with B-spline wavelets. These research efforts concentrate on boundary representation of molecules mainly for visualization, while model construction itself is not considered.

In order to support material design and analysis, computational models need to accommodate the need of model construction at multiple levels from atomic to molecular, meso, and bulk scales. Traditional boundary representation of objects is not efficient for geometric modeling at nano scales. Creation of parametric models for multi-scale uses beyond simple seamless zooming is important.

Recently, hyperbolic surfaces have attracted the attention of physicists, chemists, and biologists. Hyperbolic geometry commonly exists in natural shapes and structures. Among various hyperbolic surfaces, minimal surfaces are the most studied. Minimal surfaces are those with mean curvature of zero. If a minimal surface has space group symmetry, it is periodic in three independent directions. Triply periodic





(a) Linde A zeolite structure and TPMS P-surface.

(b) Faujasite zeolite structure and TPMS D-surface.

Fig. 1. Zeolite structures fit TPMS's [11].



Fig. 2. The zero potential surface of CsCl is close to TPMS P surface [10].

minimal surface (TPMS) is of special interest because it appears in a variety of physical structures such as silicates, bicontinuous mixtures, lyotropic colloids, detergent films, lipid bilayers, and biological formations.

#### 2.2. Minimal surface in atomistic scale

Minimal surfaces appear in atomistic scale in a very natural way. For example, TPMS's can be found in various natural or man-made crystal structures such as zeolite sodalite and perovskite-type structures [7]. As shown in Fig. 1, Linde A and faujasite zeolite structures nicely fit to one side of TPMS P and D minimal surfaces. Consider an array of electrostatic point charges arranged in different crystallographic symmetries. The surfaces of zero electrostatic potential are very close to periodic minimal surfaces such as TPMS P surface (e.g. CsCl), D surface (e.g. NaTl), and I-WP (e.g. BaCuO<sub>2</sub>) [8]. Fig. 2 shows the zero potential surface of CsCl structure, which shares the same topology and symmetry of TPMS P surface. The electron localization distribution functions also show the shape of TPMS G surfaces [9]. Based on a salient variable — curvature, over 20 years' scientific exploration of shapes in nature is summarized in a recent book of Hyde et al. [10].

Besides the beauty of periodic property, TPMS's are efficient partitioners of congruent spaces. They allow very high surfaceto-volume ratios compared to other membrane packing, which is a desirable chemical property such as in enzyme design. In addition, they offer regular networks that define labyrinths with easily accessible positions, as shown in the next section.



Fig. 3. The X-ray image reveals TPMS P surface symmetry in sea-urchin *Cidaris rugosa*.



(a) Texture of lung lavage.



(b) CLP-minimal surface model of the alveolar surface.

Fig. 4. Human lung alveoli epithelial cells have a total surface area of  $100 \text{ m}^2$  [17].

#### 2.3. Minimal surface in meso scale

Minimal surface structures are found in macromolecules. Luzzati and Spegt [12] first discovered the intricate interconnected triply periodic network domain structure in strontium soap. Donnay and Pawson [13] revealed that the interface between single calcite crystals and amorphous organic matter in the skeletal element in sea urchins is described by TMPS *P* surface, as shown in Fig. 3. TPMS-like structures are found in lyotropic liquid crystals [14], cubic phase of lipid bilayer in sunflower oil [15], and soluble proteins in lipid–protein–water phases [16]. Recently, Larsson et al. [17] report that lung alveolar surface follows the CLP surface structure, as shown in Fig. 4.

In a copolymer environment, a necessary condition for equilibrium is that the interfacial energy is minimized and



(a) [001] projection.

(b) [111] projection

Fig. 5. Micrographs from polystyrene–polyisoprene copolymer, compared with computer-simulated images of TPMS D surface in bottom-right corners [18].



(a)  $B_{20}S_{39}V_{41}^{126}$  and  $S_{45}V_{55}^{76}$  volume ratio 75/25.

(b)  $B_{20}S_{39}V_{41}^{126}$  and  $V_{58}C_{42}^{59}$  volume ratio 50/50.

300 nm

Fig. 6. Self-assembly of block copolymer exhibits gyroid morphology [23].

the interface has constant mean curvature. TPMS's have been observed in systems of emulsions and biological structures, such as star [18] and diblock polymers [19], as in Fig. 5. TPMS's can model double-diamond, gyroid, and other mean-curvature morphologies appearing in selfassembly of organic–inorganic composites [20], triblock copolymer [21], and water–oil multi-continuous phases [22]. Recently, double-gyroid surfaces are used to study core–shell gyroid morphology [23] in triblock copolymer, as in Fig. 6.

The ubiquity of hyperbolic surfaces appearing in both atomic and meso scales naturally distinguishes them as excellent candidates for multi-scale surface modeling. They provide good analytic representations of geometry with complex topology, including extremely porous structures. The belief behind multi-scale geometric modeling is that since nature is manifested by geometry, geometry is the nature. Compared to geometry in nature, regularly used engineering shapes are far too simple. It is easy to model those shapes in Euclidean space, and engineers are used to thinking in the Euclidean world. Nevertheless, some seemingly complex geometries can also be built efficiently in non-Euclidean space. In this paper, a generic periodic surface model is proposed to model both Euclidean and hyperbolic geometries. Investigating new surface-based geometric modeling methods for periodic and porous nano structures is the main goal.

# 3. Periodic surface model

A periodic surface can be generally defined as

$$\phi(\mathbf{r}) = \sum_{k=1}^{K} A_k \cos[2\pi (\mathbf{h}_k \cdot \mathbf{r})/\lambda_k + p_k] = C$$
(1)

where **r** is the location vector in Euclidean space,  $\mathbf{h}_k$  is the *k*th lattice vector in reciprocal space,  $A_k$  is the magnitude factor,  $\lambda_k$  is the wavelength of periods,  $p_k$  is the phase shift, and *C* is a constant. Specific periodic structures and phases can be constructed based on the implicit form.

#### 3.1. Approximation of TPMS

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With a generic and simpler form, periodic surfaces can approximate TPMS's and zero equipotential surfaces very well [24]. TPMS's have a precise parametric form, known as the Weierstrass formula

$$\begin{cases} x = \operatorname{Re} \int_{\omega_0}^{\omega_1} e^{i\theta} (1 - \omega^2) R(\omega) d\omega \\ y = \operatorname{Im} \int_{\omega_0}^{\omega_1} e^{i\theta} (1 + \omega^2) R(\omega) d\omega \\ z = -\operatorname{Re} \int_{\omega_0}^{\omega_1} e^{i\theta} (2\omega) R(\omega) d\omega \end{cases}$$
(2)

where  $\omega$  is a complex variable,  $\theta$  is the so-called Bonnet angle, and  $R(\omega)$  is the function which varies for different surfaces. For example, for TPMS *P*, *D* and *G* surfaces,  $R(\omega) = 1/\sqrt{1-14\omega^4 + \omega^8}$ . Compared to the parametric TPMS form, the periodic surface has a much simpler and unified representation.

Viewed from the multi-dimensional control parameter space, the geometric shape of a periodic surface is specified by a *periodic vector* 

$$\mathbf{V} = \langle \mathbf{A}, \mathbf{H}, \mathbf{P}, \mathbf{\Lambda} \rangle_{K \times 6} \tag{3}$$

where  $\mathbf{A} = [A_k]_{K \times 1}$ ,  $\mathbf{H} = [\mathbf{h}_k]_{K \times 3}$ ,  $\mathbf{P} = [p_k]_{K \times 1}$ , and  $\mathbf{\Lambda} = [\lambda_k]_{K \times 1}$  are row concatenations of magnitudes, reciprocal lattice vectors, phases, and period lengths respectively. Table 1 lists some examples of periodic surface models that approximate TPMS's, including *P*-, *D*-, *G*-, and *I*-*WP* cubic morphologies that are frequently referred to in chemistry and polymer literature. In the rest of the paper, we refer to *P*, *D*, *G*, and *I*-*WP* surfaces as periodic surfaces, unless specified with the term of TPMS.

Besides the cubic morphologies, other meso phase structures of spherical micelles, lamellar, rodlike hexagonal phases can also be modeled by periodic surfaces. Table 2 lists some of the examples. Notice that some of these structures are in the domain of Euclidean geometry, which shows the generality of the periodic surface model.

# 3.2. Operations on periodic zero surface

A periodic surface partitions 3D space into two congruent subspaces. If we consider a periodic zero surface  $\phi(\mathbf{r}) = 0$ , two sides of the zero surface have opposite (+ and -) signs of function evaluation. Two types of operations on periodic zero surfaces can be used to construct complex shapes. One is volume-oriented, such as *union*, *difference*, and *exclusive or*, the other is surface-oriented, including *intersection*, *modulation*, and *convolution*.

# 3.2.1. Union

Given surfaces  $\phi_1(\mathbf{r}) = 0$  and  $\phi_2(\mathbf{r}) = 0$ , the union operations are defined as  $\phi_1 \cup \phi_2 := \min(\phi_1, \phi_2)$  and  $\phi_1 \cup \phi_2 := \max(\phi_1, \phi_2)$ . The union operation  $\cup^-$  merges two labyrinth volumes with - sign, while  $\cup^+$  merges those with +sign. Fig. 7 illustrates the union operations. Surface  $\phi_A(\mathbf{r}) = 0$ is defined by periodic vector

$$\mathbf{V}_{A} = \left\langle \begin{bmatrix} 1\\1\\1\\1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0\\0 & 1 & 0\\0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 0\\0\\0\\0 \end{bmatrix} \begin{bmatrix} 1\\1\\1\\1 \end{bmatrix} \right\rangle \tag{4}$$

as in Fig. 7(a). Surface  $\phi_B(\mathbf{r}) = \phi_A(\mathbf{r} + [0.3, 0.3, 0]^T) = 0$  has a distance shift from  $\phi_A(\mathbf{r}) = 0$ , as in Fig. 7(b). The results of two union operations are shown in Fig. 7(c) and (d). Union operation changes the volume ratio of two sides.

# 3.2.2. Difference

Given surfaces  $\phi_1(\mathbf{r}) = 0$  and  $\phi_2(\mathbf{r}) = 0$ , the difference operations are defined as  $\phi_1 \setminus \phi_2 := \min(-\phi_1, \phi_2) = \max(\phi_1, -\phi_2)$  and  $\phi_1 \setminus \phi_2 := \min(\phi_1, -\phi_2) = \max(-\phi_1, \phi_2)$ . The difference operation  $\setminus$  gives the volume difference of two labyrinths with - sign, while  $\setminus$  returns the volume difference with + sign. They are illustrated in Fig. 9(e) and (f).

# 3.2.3. XOR

Given surfaces  $\phi_1(\mathbf{r}) = 0$  and  $\phi_2(\mathbf{r}) = 0$ , the XOR is defined as  $\phi_1 \tilde{\vee} \phi_2 := \phi_1 \cdot \phi_2$ . The XOR is an exclusive or operation on volumes with + and - signs. It can also be looked on as surface union by which two periodic zero surfaces merge into one.

# 3.2.4. Intersection

Given surfaces  $\phi_1(\mathbf{r}) = 0$  and  $\phi_2(\mathbf{r}) = 0$ , the intersection is defined as  $\phi_1 \wedge \phi_2 := (\phi_1)^2 + (\phi_2)^2$ . Analytically, intersection of two periodic surfaces will be curves in  $E^3$ , and intersection of three periodic surfaces gives points.

#### 3.2.5. Modulation

Given surfaces  $\phi_1(\mathbf{r}) = 0$  and  $\phi_2(\mathbf{r}) = 0$ , the modulate operation is defined as  $\phi_1 \oplus_m \phi_2 := \phi_1 + \phi_2/m$ , where  $\phi_1$  is the main surface,  $\phi_2$  is the modulating surface, and *m* is the modulation index. The modulate operation adds fine features of the modulating surface onto the main surface. Fig. 8 illustrates the effect of modulate operation, where surface  $\phi_A(\mathbf{r}) = 0$ is a *P* surface with the periodic vector in Eq. (4) and surface  $\phi_C(\mathbf{r}) = 0$  is a *G* surface with the periodic vector

Morphology and structure	Periodic surface model	Surface
Р	$\phi(\mathbf{r}) = A_P \left[ \cos(2\pi x/\lambda_x) + \cos(2\pi y/\lambda_y) + \cos(2\pi z/\lambda_z) \right] = 0$ $\mathbf{A}^{\mathrm{T}} = \begin{bmatrix} 1 & 1 & 1 \end{bmatrix}  \mathbf{H}^{\mathrm{T}} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}  \mathbf{P}^{\mathrm{T}} = \begin{bmatrix} 0 & 0 & 0 \end{bmatrix}$	
D	$\phi(\mathbf{r}) = A_D \begin{bmatrix} \cos(2\pi x/\lambda_x) \cos(2\pi y/\lambda_y) \cos(2\pi z/\lambda_z) \\ -\sin(2\pi x/\lambda_x) \sin(2\pi y/\lambda_y) \sin(2\pi z/\lambda_z) \end{bmatrix} = 0$ $\mathbf{A}^{\mathrm{T}} = \begin{bmatrix} 1 & 1 & 1 & -1 & 1 & -1 \end{bmatrix}$ $\mathbf{H}^{\mathrm{T}} = \begin{bmatrix} 1 & 1 & 1 & 1 & -1 & -1 & -1 \\ -1 & -1 &$	
G	$\mathbf{P}^{\mathrm{T}} = \begin{bmatrix} 0 & 0 & 0 & \pi/2 & \pi/2 & \pi/2 & \pi/2 \end{bmatrix}$ $\phi(\mathbf{r}) = A_G \begin{bmatrix} \sin(2\pi x/\lambda_x)\cos(2\pi y/\lambda_y) + \sin(2\pi y/\lambda_y)\cos(2\pi z/\lambda_z) \\ +\sin(2\pi z/\lambda_z)\cos(2\pi x/\lambda_x) \end{bmatrix} = 0$ $\mathbf{A}^{\mathrm{T}} = \begin{bmatrix} 1 & 1 & 1 & 1 & -1 \end{bmatrix}  \mathbf{H}^{\mathrm{T}} = \begin{bmatrix} -1 & -1 & 0 & 0 & -1 & -1 \\ -1 & 1 & -1 & -1 & 0 & 0 \\ 0 & 0 & -1 & 1 & -1 & 1 \end{bmatrix}$ $\mathbf{P}^{\mathrm{T}} = \begin{bmatrix} \pi/2 & \pi/2 & \pi/2 & \pi/2 & \pi/2 \end{bmatrix}$	
I-WP	$\phi(\mathbf{r}) = A_I \begin{bmatrix} 2\cos(2\pi x/\lambda_x)\cos(2\pi y/\lambda_y) + 2\cos(2\pi y/\lambda_y)\cos(2\pi z/\lambda_z) \\ +2\cos(2\pi z/\lambda_z)\cos(2\pi x/\lambda_x) \\ -\cos(4\pi x/\lambda_x) - \cos(4\pi y/\lambda_y) - \cos(4\pi z/\lambda_z) \end{bmatrix} = 0$ $\mathbf{A}^{\mathrm{T}} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & -1 & -1 & -1 \end{bmatrix}$ $\mathbf{H}^{\mathrm{T}} = \begin{bmatrix} 1 & 1 & 0 & 0 & 1 & 1 & 2 & 0 & 0 \\ -1 & 1 & 1 & 1 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & -1 & 1 & -1 & 1 & 0 & 0 & 2 \end{bmatrix}$ $\mathbf{P}^{\mathrm{T}} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$	

The modulated surface  $(\phi_A \oplus_m \phi_C)(\mathbf{r}) = 0$  with different modulation indices m = 1.0, 2.0, 5.0, and 10.0 is shown in Fig. 8(c), (d), (e), and (f) respectively.

# 3.2.6. Convolution

Given surfaces  $\phi_1(\mathbf{r}) = 0$  and  $\phi_2(\mathbf{r}) = 0$ , the convolute operation is defined as  $\phi_1 \otimes \phi_2(\mathbf{r}) := \iiint_D \phi_1(\mathbf{q})\phi_2(\mathbf{r} - \mathbf{q})d\mathbf{q}$ in the domain  $\mathbb{D}$ . The convolute operation can be looked as the inverse operation of modulate. Convolution has the effect of filtering and smoothing. As illustrated in Fig. 9, surface  $\phi_B(\mathbf{r}) = \phi_A(\mathbf{r} + [0.3, 0.3, 0]^T) = 0$  is a *P* surface with the periodic vector in Eq. (4). Surface  $\phi_C(\mathbf{r}) = 0$  is a *G* surface with the periodic vector in Eq. (5). Surface  $\phi_D(\mathbf{r}) = 0$  is generated by modulation. If surface  $\phi_D(\mathbf{r}) = 0$  is convoluted with the surface  $\phi_A(\mathbf{r}) = 0$ , the fine features of  $\phi_C(\mathbf{r}) =$ 0 are filtered out and the original surface  $\phi_B(\mathbf{r}) = 0$  is recovered.

In multi-scale surface representation, modulation and convolution operations form the basis of seamless zooming.

Geometric details in smaller scales can be added with modulation as zoomed in. When zoomed out, details are filtered out with convolution.

Periodic surfaces exhibit infinitely periodic thus scalable properties. With simple mathematic representation, they inherently represent continuous labyrinth space and high surface–volume ratio geometry with porous features, which universally appear in natural structures. With the basic periodic surface skeleton, atomistic structures can be constructed based on mapping from 2D hyperbolic space to 3D Euclidean space, which is a tiling process. In the next section, a symmetric tiling method for crystal construction is presented.

# 4. Symmetric tiling

Tiling is periodic subdivision of space into bounded and connected regions. The problem of constructing molecules and crystals is indeed tiling in Euclidean 3D space. Instead of filling 3D space directly, an indirect approach [25,26] is to tile the

Table 2	
Periodic surface representation of mesophase structures	

Morphology and structure	Periodic surface model	Surface
Lamellar	$\mathbf{A}^{\mathrm{T}} = \begin{bmatrix} 1 \\ \\ 0 \\ 1 \end{bmatrix}$ $\mathbf{P}^{\mathrm{T}} = \begin{bmatrix} 0 \\ \\ 1 \end{bmatrix}$ $\mathbf{A}^{\mathrm{T}} = \begin{bmatrix} 1 \end{bmatrix}$	
Rod	$\mathbf{A}^{\mathrm{T}} = \begin{bmatrix} 1 & 1 & 3 & 3 & 3 \end{bmatrix}$ $\mathbf{H}^{\mathrm{T}} = \begin{bmatrix} 1 & 0 & -1 & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ $\mathbf{P}^{\mathrm{T}} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ $\mathbf{\Lambda}^{\mathrm{T}} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \end{bmatrix}$	
Sphere	$\mathbf{A}^{\mathrm{T}} = \begin{bmatrix} 1 & 1 & 1 & 3 & 3 & 3 & 9 \end{bmatrix}$ $\mathbf{H}^{\mathrm{T}} = \begin{bmatrix} 1 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & -1 & 0 \end{bmatrix}$ $\mathbf{P}^{\mathrm{T}} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$	
Membrane or mesh	$\mathbf{\Lambda}^{\mathrm{T}} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 &$	
	$\mathbf{\Lambda}^{\mathrm{T}} = \begin{bmatrix} 1 & 0.5 & 0.5 & 0.5 & 0.5 & 0.5 & 0.5 & 0.5 \end{bmatrix}$	

2D hyperbolic space first and then create a mapping from 2D hyperbolic space  $H^2$  to 3D Euclidean space  $E^3$ . Inorganic chemists have recognized that a symmetric pattern is the centrality in understanding condensed atomic, molecular, and colloidal aggregates. A broad spectrum of Euclidean structures can result from a single hyperbolic one with symmetric tiling.

Hyperbolic geometry satisfies all of Euclid's postulates except the parallel postulate: for any straight line L and any point P not on L, there are infinitely many other straight lines that pass through the point P and do not intersect the line L. These lines are all parallel to L. The Poincaré disk is the most used 2D hyperbolic conformal model. As shown in Fig. 10, in a Poincaré's hyperbolic disk of  $H^2$ , a line is represented as an arc whose ends are perpendicular to the disk's boundary, which represents infinity. Two arcs which do not meet correspond to parallel lines in  $H^2$ . For example,  $l_1$ ,  $l_2$ ,  $l_3$ , and  $l_4$  are all parallel to each other in Fig. 10(a). Any point on the disk has its correspondence on an infinitely periodic surface. As shown in Fig. 10(b), three points a, b, and c in  $H^2$  are mapped to A, B, and C in  $E^3$  respectively. With the mapping of atom locations from  $H^2$  to periodic surfaces, large crystal structures can be constructed with specified period. Increasing the number of periodic cycles results in a large volume of materials with atoms or particles filling the space. Fig. 11 shows an example structure from Fig. 10 with two different particle sizes. Notice that one single surface passes through all particles. The surface delineates the loci of particles.

To tile a periodic surface, two approaches can be taken. One is tiling by surface intersection, in which tiling is an intersection by two or three periodic surfaces, the other is tiling by surface modulation, in which tiling is the intersection between the main surface and the modulated surface.

#### 4.1. Surface tiling by intersection

The locations of atoms or particles in  $E^3$  space can be determined by their simultaneous appearances in three or more  $H^2$  spaces. Tiling surface  $\phi_1(\mathbf{r}) = b_1$  with surfaces  $\phi_2(\mathbf{r}) = b_2$  and  $\phi_3(\mathbf{r}) = b_3$  is to solve equations

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Fig. 7. Union and difference operations on periodic surfaces (red and yellow colors indicate + and - sides of the surfaces respectively). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)



 $\begin{cases} \phi_1(\mathbf{r}) = b_1 \\ \phi_2(\mathbf{r}) = b_2 \\ \phi_3(\mathbf{r}) = b_3 \end{cases}$ 

which is equivalent to

(6) 
$$\phi(\mathbf{r}) = [\phi_1(\mathbf{r}) - b_1]^2 + [\phi_2(\mathbf{r}) - b_2]^2 + [\phi_3(\mathbf{r}) - b_3]^2 = 0.$$
 (7)

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Fig. 9. An example of convolution as the inverse of modulation.

and





$$\mathbf{V}_{X2} = \left\langle \begin{bmatrix} 1\\1\\1\\1\\1 \end{bmatrix} \begin{bmatrix} 1 & -1 & -1\\1 & 1 & -1\\1 & 1 & -1\\1 & 1 & 1 \end{bmatrix} \begin{bmatrix} \pi/2\\ -\pi/2\\ -\pi/2\\ \pi/2 \end{bmatrix} \begin{bmatrix} 2\\2\\2\\2\\2 \end{bmatrix} \right\rangle.$$
(9)

(a) Poincaré disk.

(b) Periodic surface in 3D Euclidean space.

Fig. 10. Mapping from Poincaré's disk  $H^2$  to periodic surface in  $E^3$ .



Fig. 11. Crystal constructed from a tiled P surface in Fig. 10.

For example, the periodic sodalite framework in Fig. 12(a) can be naturally generated by the intersection of one *P* surface and two grid surfaces with periodic vectors

$$\mathbf{V}_{X1} = \left\langle \begin{bmatrix} 1\\1\\1\\1\\1 \end{bmatrix} \begin{bmatrix} 1 & -1 & -1\\1 & -1 & 1\\1 & 1 & -1\\1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 0\\0\\0\\0 \end{bmatrix} \begin{bmatrix} 1\\1\\1\\1\\1 \end{bmatrix} \right\rangle$$
(8)

# 4.2. Surface tiling by modulation

In the modulation tiling approach, the main surface is modulated by high frequency surfaces. The intersection curves between the modulated surface and the original main surface naturally divide the surface with symmetric patterns. For instance, if a *P* surface  $\phi_A(\mathbf{r}) = 0$  with the periodic vector in Eq. (4) is modulated by a grid surface  $\phi_X(\mathbf{r}) = 0$  with the periodic vector

$$\mathbf{V}_{X}(n) = \left\langle \begin{bmatrix} 1\\1\\1\\1 \end{bmatrix} \begin{bmatrix} n & -n & -n\\n & -n & n\\n & n & -n\\n & n & n \end{bmatrix} \begin{bmatrix} 0\\0\\0\\0 \end{bmatrix} \begin{bmatrix} 1\\1\\1\\1\\1 \end{bmatrix} \right\rangle$$
(10)

where *n* ranges from 1 to 10. When the modulation index m = 20, the tiled *P* surfaces are shown in Fig. 13. Notice that the intersection between the two surfaces generates periodic and self-intersecting curves, upon which cages and crystal lattices can be built. Intersecting with a third surface will determine the location of particles.

# 5. Surface enclosure

Instead of being looked at as *loci* of atoms and particles as in tiling, periodic surfaces are regarded as isosurfaces of energy or potential in surface enclosure. Atoms or particles are enclosed by periodic surfaces, and the *foci* of surfaces





(a) Sodalite lattice of 14-sided cages. Vertices correspond to Si (Al) and edges represent Si–O–Si (Si–O–Al) bonds.





(e) Surface intersection.

Fig. 12. Tiling by intersection of P surface with grid surfaces to create sodalite framework.

determine positions of particles. Surfaces then are energy or potential envelopes of particles. For instance, in Fig. 14, periodic P- or D-surface divides 3D space into two congruent labyrinth subspaces. The Body-Centered Cubic (BCC) crystal structure is easily constructed by searching foci of P- or Dsurfaces. Complex structures can be built with careful selection of potential envelopes and periodicity.

Given a periodic vector such as the potential envelope, the positions of surface foci can be determined. Instead of directly using maximum and minimum potentials in Euclidean space, we can search foci based on divergence of potential field intensity

$$\nabla^2 \phi(\mathbf{r}) = \nabla \cdot \mathbf{F}(\mathbf{r}) = \rho(\mathbf{r}) \tag{11}$$

where  $\mathbf{F}(\mathbf{r})$  is the potential field intensity, and  $\rho(\mathbf{r})$  can be looked on as the charge density of particles.  $\rho(\mathbf{r})$  is close to zero in inter-particle space and tends to increase or decrease as it approaches particle positions. Foci searching based on  $\rho(\mathbf{r})$  also increases the robustness of searching with possible presence of noise compared to searching directly on  $\phi(\mathbf{r})$ . Fig. 15 shows an example of using foci enclosure to build the atomic structures of BaSi<sub>2</sub>. The cubic and layer phases can be constructed based on periodic surface envelopes, which are a *D* surface and a mesh surface with the vector

for two phases respectively. Positions of Si are indicated by red dots and Ba are in blue. Foci surfaces provide a good connection between physics and geometry in the form of potential and field.

#### 6. Discussion

The periodic surface modeling enables rapid geometry construction for simulation and design validation purpose. It provides flexible geometric models to represent natural shapes and man-made structures in atomistic, molecular, and meso scales, including crystals, polymers, and porous composites. This model provides a simple yet versatile solution to lack of model construction methods for nano product design, as porous structure is functionally important in various applications. For example, the partition of space in an organelle enables cells to control the concentrations of various molecules and their transport across bilayers. Surfactant can be used as a template for polymerization reactions and produce nano products such as mesoporous silica molecular sieves, or hydrogels with well defined pore sizes and shapes for contact lenses, etc.

The simplicity of implementation is another advantage of the periodic surface modeling. A discrete approach can be taken to create the implicit surface models. Periodic surfaces are evaluated at lattice points within a periodic unit of interest, and isosurfaces are generated to approximate and visualize the surfaces. Periodic zero surface operations defined in Section 3.2 can be implemented based on the approximation of finite grids within a periodic unit. The volume integration of the convolute operation can be implemented based on Fast Fourier Transform



Fig. 13. Tiling P surface with grid surface modulation.



Fig. 14. BCC crystal structures enclosed by periodic P and D surfaces.

(FFT). Because of the FFT's dimensional separability, the time complexity of the 3D convolution is  $O(N^3 \log N)$  where N is the number of grid points in one dimension within a periodic volume unit. Because of the periodic boundary condition, special attention is needed in calculating gradients and divergence in model construction with surface enclosure.

Topology representation in periodic surfaces needs further study in future research. In this paper, only the geometry of surface structure is discussed without consideration of topology, although surface enclosures can be used to represent envelopes of chemical bonds. There are some challenges in capturing nano-scale topology. Various intra- and intermolecular forces exist with different strengths and ranges. The



(a) BaSi<sub>2</sub> structures in cubic phase and layer phase.



(b) Corresponding foci surfaces of Si envelope.

Fig. 15. Foci search from surface enclosure of  $BaSi_2$ . (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

angles of covalent bonds play important roles in structural energy distribution. The process of bond formation and breaking is a dynamic equilibrium in nature. Thus, connectivity between atoms is dynamic and complex. Other research issues in the future include modeling nano structures with uncertainty and structural defects, as well as aperiodic and fractal geometries which have intrinsic connections to periodic geometries.

# 7. Conclusion

In this paper, a new periodic surface modeling scheme for computer aided nano design is proposed. Based on periodic hyperbolic surfaces, geometry of thousands of particles can be built efficiently at the molecular scale. It takes a generic approach to explore symmetric tiling and packing of loci surfaces in 2D hyperbolic space and subsequently mapping into conventional 3D Euclidean space. The surface enclosure method provides a physics-based approach to construct crystals based on foci searching. At the meso scale, morphology of polymer and macromolecule can also be represented. Associated surface and volume operations are defined to support model creation. This new scheme helps to model periodic and porous structures for material design at atomic, molecular, and meso scales.

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