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Issue Article

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METHOD FOR GENERATION OF NEW POROUS MATERIALS BASED ON TRIPLY PERIODIC SURFACES

Abstract: *A new method is proposed for generation of porous materials, which is based on triply periodic surfaces (TPS) derived from topological network representation of crystal structures of chemical compounds. A model of the porous material based on the sodalite crystal structure is generated, samples of the material are manufactured by 3D printing.*

Key words: *triply periodic surfaces, additive manufacturing, porous material.*

Language: *English*

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Introduction

Modern technologies widely use materials with porous structure of various types and dimensions [1]. An important group of such materials, which attracted attention in the last years, is based on smooth triply periodic surfaces (TPS) with diverse topological and geometrical structure [2, 3]. The interest to these materials is primarily caused by their thermal-conductive, electrical-conductive, acoustic, and vibration-isolating properties [4, 5], as well as by their ability to adsorb strain energy [6–11]. Filling pores with the materials to be different from the skeleton base material enables one to fabricate new composite materials and metamaterials with wide range and considerable anisotropy of physical properties. The mentioned features together with the Additive Manufacturing (AM) technology make the TPS materials an indispensable part of modern engineering solutions and thus are a subject of intense theoretical and experimental studies.

However, the number of TPSs currently used in the development of porous materials is quite limited, and the task of generating new TPSs is vital [12]. In this paper, we describe a new method for the generation of TPS-based porous materials derived from topological network representation of crystal structures of chemical compounds, in particular, zeolites [13, 14]. The theoretical background of this method is described in detail in [15]. This approach enables one to generate an unlimited number of TPSs and the corresponding porous materials using the *ToposPro* program package [16]. After a certain thickness is attributed to the surface, it can be 3D printed, and its physical properties can be explored with a computer-aided engineering (CAE) system like the ANSYS software [17], and studied experimentally.

The procedure for porous material generation based on triply periodic frames structured from natural crystals

A new *network approach* for generating triply periodic surfaces was developed, which is based on crystal structures of chemical compounds. This approach includes the following steps, all of which can be performed with *ToposPro*:

(i) Constructing a periodic net for a given crystal structure by determining interatomic bonds with the universal *Domains* algorithm [18] (Fig. 1 top left).

(ii) Building *natural tiling* for the net following a rigorous algorithm [19]. The natural tiling consists of polyhedral cages (*natural tiles*, Fig. 1 top right), which are confined by rings of the net (natural tile faces). The natural tiles possess an important property: they are minimal cages in the structure, and any other cage can be assembled from several natural tiles.

(iii) Generating TPSs from the natural tiling by the enumeration of all such ways of removing natural tile faces when the set of remaining faces obeys three conditions: (a) *decoration condition*, which requires that all net vertices and edges must lie on the TPS; (b) *edge condition*, according to which any edge of the net is shared by strictly two faces from the set; (c) *vertex condition*, which states that all edges meeting at the same vertex are shared by different pairs of faces. These conditions ensure that the resulting set of faces forms a single TPS without self-crossings (Fig. 1 bottom).

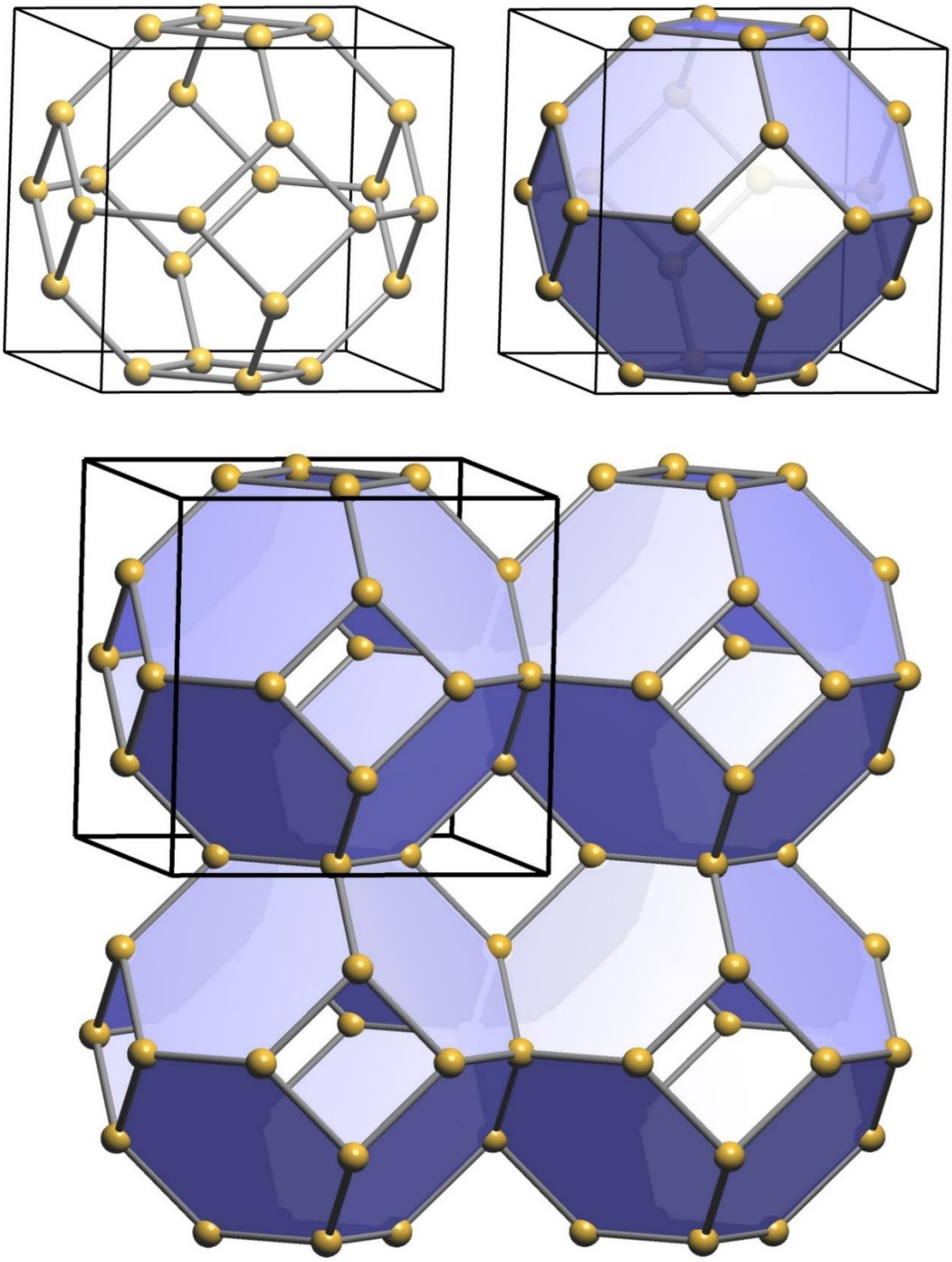

Figure 1. Zeolite sodalite (SOD) crystal structure: (top left) a fragment of periodic net in the unit cell; (top right) a natural tile confined by 4-membered and 6-membered rings of the net; (bottom) the triply periodic surface generated by removing the 4-membered rings and represented by the 6-membered facets.

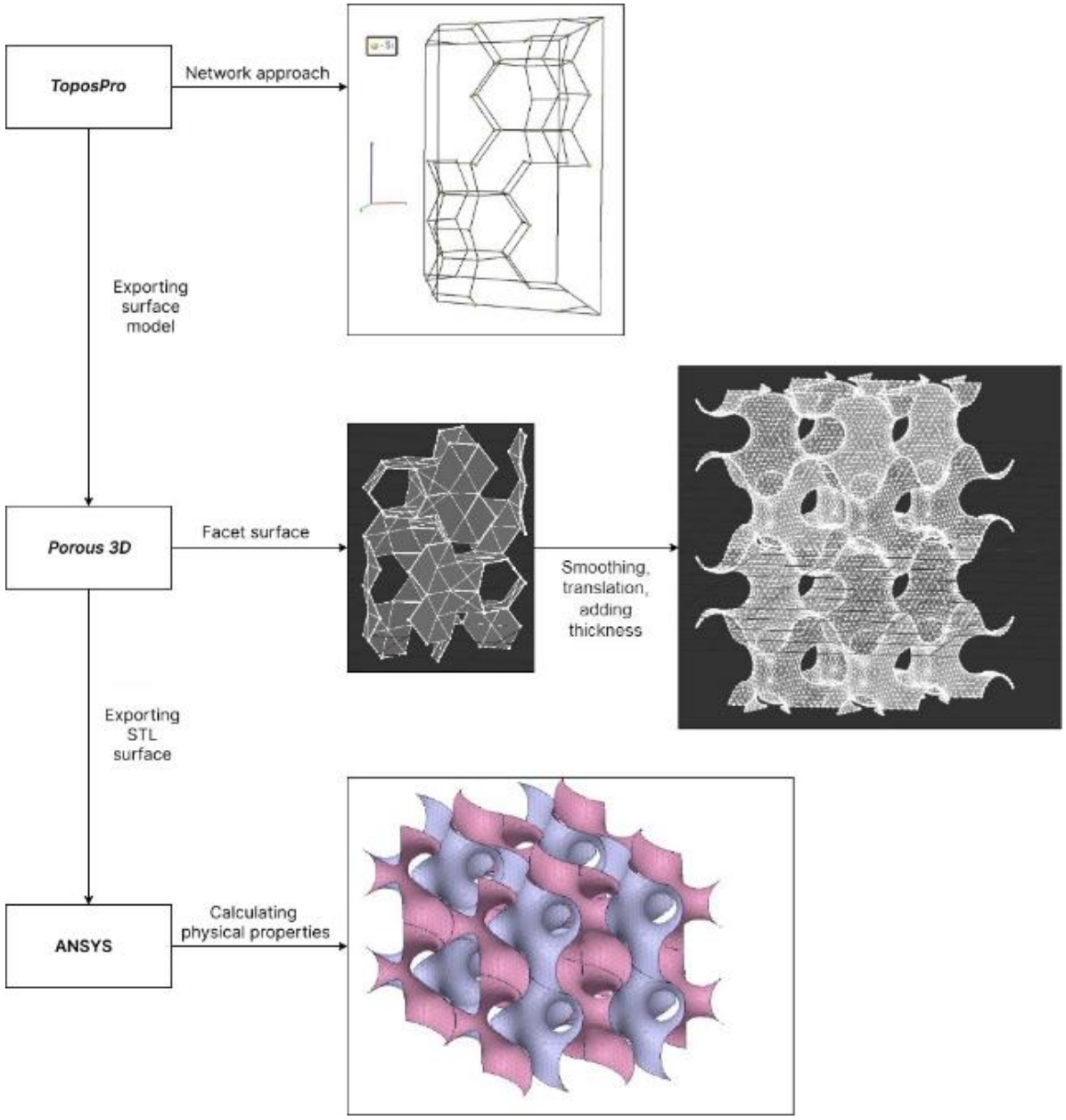

Figure 2. Schematic representation of the procedure used to generate a mathematical model of a porous material based on the AFG zeolite structure and to theoretically study its mechanical and thermal properties using *ToposPro, Porous 3D,* and ANSYS software.

The resulting TPS divides the space into two non-crossing parts (labyrinths), which can be equivalent if the TPS is minimal and balanced [20]. Geometrically, the TPS obtained in this way has a facet structure and needs smoothing to gain a minimal mean curvature. Since the number of periodic nets is infinite, and more than 800,000 of them have been stored in the *TopCryst* database [21], this approach provides an unrestricted opportunity for generation and discovering of new TPSs, which can serve as templates for porous materials and metamaterials. Some of new TPSs were obtained in [15], and a database with the mathematical models of these TPSs was created. We have used the information from this database to fabricate porous materials in this work (Fig. 2).

Let us discuss this procedure in more detail. The TPS facet model generated by *ToposPro* is output to a textual .t3g file, where the coordinates of all facets (rings) are given (Fig. 3).

```
1  AFG: 3D surface formed by rings: ◇4a, ⬢6a, ⬡6c, ⬢6d, ⬢6f
2  12.54800 (a)  12.54800 (b)  20.78900 (c)
3  90.00 (α)  90.00 (β)  120.00 (γ)
4  RING 4  a
5  0.08890  0.67060  0.37460
6  0.00350  0.75340  0.25000
7  0.24660  0.99650  0.25000
8  0.32940  0.91110  0.37460
9  ...
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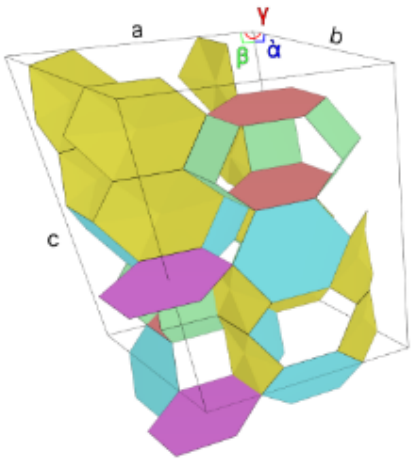

Figure 3. The .t3g-format file generated by *ToposPro* for a triply periodic surface represented by one 4-membered and four independent 6-membered rings of the periodic net obtained for the AFG zeolite crystal structure as well as dimensions and angular parameters of the unit cell.

Line 1 contains the periodic net name (AFG) and all independent (symmetry-inequivalent) rings (4a, 6a, 6c, 6d, 6f), which were used to compose the TPS.

Lines 2 and 3 specify the dimensions and angular parameters of the unit cell.

Line 4 starts the description of a TPS facet with the RING keyword followed by the size and type of the facet (4a);

Lines 5 – 8 record the coordinates of the net vertices, which form the facet; the coordinates are expressed in fractions of the unit cell dimensions.

The remaining lines are similar to lines 4 – 8 for all other facets in the unit cell.

To visualize, smooth and thicken the TPS model described in a .t3g file as well as to export the resulting smoothed and thickened model into a 3D printable STL-format file we have developed the *Porous 3D* software [22], which is based on the following algorithms.

Model translation algorithm. Obtaining an infinite TPS implies gluing boundaries of the adjacent unit cells. For this purpose, parallel translation in space in rectangular coordinate system *(x, y, z)* is implemented analytically using the following method (1):

Let *S* be the model that needs to be translated and $S(p_i)$ is a vertex of this model. To translate *S*, we need to calculate the translation matrix *T* based on the unit cell parameters *a*, *b*, *c*, α, β, γ:

$$T = \begin{pmatrix} a & b\cdot\cos(\gamma) & c\cdot\cos(\beta) \\ a\cdot\cos(\beta) & b & c\cdot\cos(\alpha) \\ a\cdot\cos(\alpha) & b\cdot\cos(\beta)\cdot\cos(\gamma) & c \end{pmatrix} = \begin{pmatrix} t_1 \\ t_2 \\ t_3 \end{pmatrix} \quad (1)$$

So, using calculated vector we can translate *S* in any direction along t_1 (2.1), t_2 (2.2), t_3 (2.3) like this:

$$t_1 : \sum_0^n S(p_i) + nt_1 \ (2.1)$$

$$t_2 : \sum_0^n S(p_i) + nt_2 \ (2.2)$$

$$t_3 : \sum_0^n S(p_i) + nt_3 \ (2.3)$$

where n is the number of models needed along translation vector (Fig. 4).

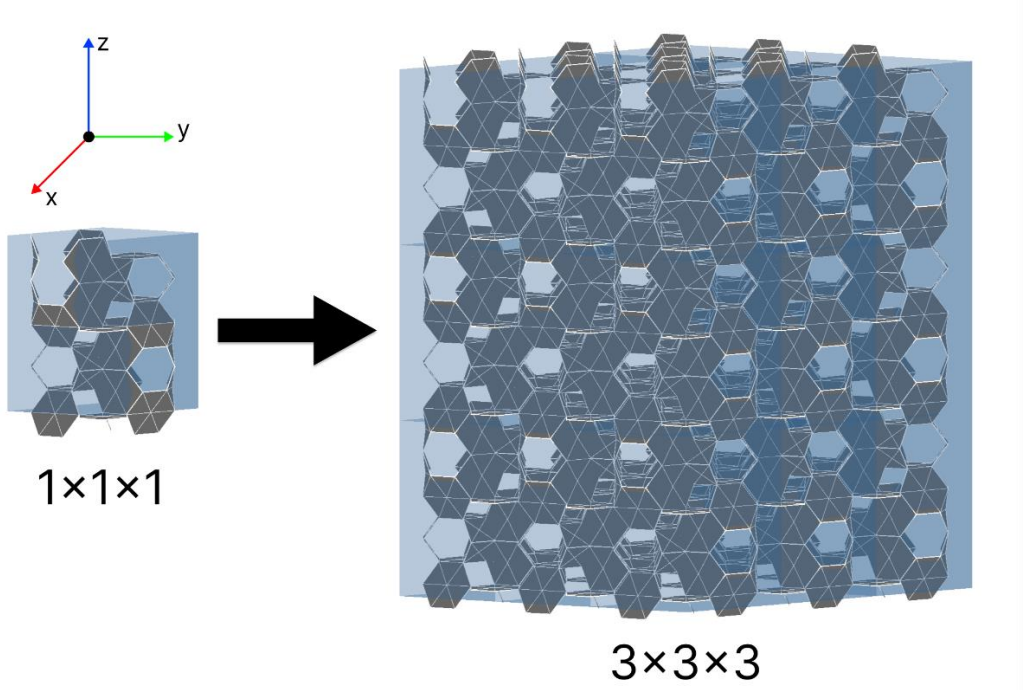

Figure 4. Translating and gluing 27 of unit cells of a TPS model generated from the AFG zeolite net. The boundaries of the internal unit cells (highlighted in cyan on the left) were removed after translating.

Facet smoothing algorithm combines Laplacian-based and optimization-based smoothing methods and minimizes the modulus of the difference between the maximum and minimum values of the mean curvatures calculated at all vertices of the surface mesh [15]. The mean curvature is calculated with the Delaunay triangulation and theory of normal cycles of differential geometry [23].

Surface thickening algorithm. Assigning thickness to a surface is made in two steps. At the first step, all points of the surface are moved along their normal vectors to a specified distance and a copy of the original surface is generated based on the moved points. At the second step, additional polygons are created to fill the gaps between the original surface and the copy to provide continuous volume.

For further investigation of physical properties of the porous material the model could be converted from STL to the Parasolid solid-state geometry format using the SpaceClaim software module of ANSYS [17].

Note that other recent studies [4, 5, 7-11, 24-26], where TPS surfaces were used for the modeling of porous materials, applied an analytical formula for constructing this TPS. Our method does not need any TPS analytical representation and, hence, we can also use those new TPSs obtained by our approach, which have no analytical description yet.

Thus, the theoretical part of our investigation included the following steps:

1. A triply periodic net is constructed using the crystallographic data on a crystal structure and *ToposPro*.
2. Facet TPSs are generated from the net with *ToposPro*, and the information on each TPS is exported into a .t3g file.
3. The data from the .t3g file are imported into *Porous 3D* and the facet TPS model is multiplied by translations, smoothed, thickened and exported into a .stl file.

The STL model could be imported to ANSYS to study thermophysical and mechanical properties of the model.

Conclusion

The new approach for generation of porous materials which based on triply periodic surfaces (TPS) is developed. The approach contains, firstly, the procedure for constructing the TPS. TPS are derived from topological network representation of crystal structures of chemical compounds in *ToposPro* software package. *ToposPro* produces surfaces bounded by various polygons, which divide the space into two non-crossing parts (labyrinths). Secondly, the resulting TPS is smoothed, taking into account the condition of minimal average curvature. At the third step, the surface is given the required thickness and it is converted into a format suitable for 3D printing and for use in applied calculation packages such as ANSYS, for example.

Developed approach provides one an unrestricted opportunity for generation and discovering of new TPSs, which can be templates for porous materials and metamaterials. A database of porous materials and tools for working with them have been created in the work.

So, the results obtained in the present paper give opportunity to state high efficiency and great opportunities of the suggested approach to generation of new porous materials as well as in theoretical and experimental studies of their physical properties.

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