New family of tilings of three-dimensional Euclidean space by tetrahedra and octahedra

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Edited* by Ronald L. Graham, University of California, La Jolla, CA, and approved May 17, 2011 (received for review April 7, 2011)

It is well known that two regular tetrahedra can be combined with a single regular octahedron to tile (complete fill) three-dimensional Euclidean space $\mathbb{R}^3$. This structure was called the "octet truss" by Buckminster Fuller. It was believed that such a tiling, which is the Delaunay tessellation of the face-centered cubic (fcc) lattice, and its closely related stacking variants, are the only tessellations of $\mathbb{R}^3$ that involve two different regular polyhedra. Here we identify and analyze a unique family comprised of a noncountably infinite number of periodic tilings of $\mathbb{R}^3$ whose smallest repeat tiling unit consists of one regular octahedron and six smaller regular tetrahedra. We first derive an extreme member of this unique tiling family by showing that the "holes" in the optimal lattice packing of octahedra, obtained by Minkowski over a century ago, are congruent tetrahedra. This tiling has 694 distinct concave (i.e., nonconvex) repeat units, 24 of which possess central symmetry, and hence is distinctly different and combinatorically richer than the fcc tetrahedra-octahedra tiling, which only has two distinct tiling units. Then we construct a one-parameter family of octahedron packings that continuously spans from the fcc to the optimal lattice packing of octahedra. We show that the "holes" in these packings, except for the two extreme cases, are tetrahedra of two sizes, leading to a family of periodic tilings with units composed four small tetrahedra and two large tetrahedra that contact an octahedron. These tilings generally possess 2,068 distinct concave tiling units, 62 of which are centrally symmetric.

space-filling | nonoverlapping solids | polytopes

Tilings have intrigued artists, architects, scientists, and mathematicians for millenia (1). A "tiling" or "tessellation" is a partition of Euclidean space $\mathbb{R}^d$ into closed regions whose interiors are disjoint. Tilings of space by polyhedra are of particular interest. Certain periodic polyhedral tilings are intimately connected to lattices (2–5) and crystal states of matter (6), and can provide efficient meshings of space for numerical applications (e.g., quadrature and discretizing partial differential equations) (7). Polyhedral tilings arise in the structure of foams and Kelvin's problem (3, 8, 9, 10). Remarkably, crystalline forms of DNA can be generated by using specifically constructed mathematical tiling analogs (11). Some aperiodic tilings of Euclidean space underlie quasicrystals (12, 13), which possess forbidden crystallographic symmetries, and glassy states of matter (14). Tilings of high-dimensional Euclidean space also have important applications in communications, cryptography, information theory, and in the search for gravitational waves (2, 15).

Tilings of two-dimensional (2D) Euclidean space $\mathbb{R}^2$ by regular polygons have been widely used since antiquity. Kepler was the first to provide a systematic mathematical treatment of 2D tiling problems in his book entitled *Harmonices Mundi* (16). Kepler showed that there are just 11 uniform tilings of $\mathbb{R}^2$ with regular polygons. A tiling is *uniform* if the symmetry group of the tiling acts transitively on its vertices. The 11 uniform tilings of $\mathbb{R}^2$ consist of the three regular tilings composed of regular polygons (regular triangles, squares, and hexagons, see Fig. 1) and eight semiregular (Archimedean) tilings, six of which are made of two

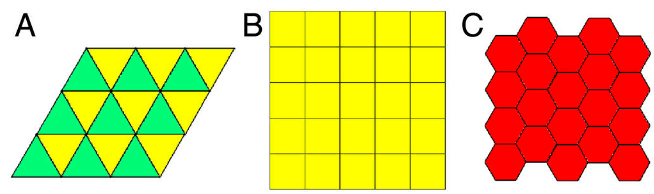

Fig. 1. The three regular tilings of the plane: (*A*) A portion of the tiling by triangles with a fundamental cell containing two triangles with two different orientations (shown by different shadings). (*B*) A portion of the tiling by squares. (*C*) A portion of the tiling by hexagons.

regular polygons and the remaining two of which are made of three regular polygons.

The analogous classification of the tilings of three-dimensional (3D) Euclidean space $\mathbb{R}^3$ is much more difficult and has not yet been completely solved to date. However, we do know that high-symmetry tilings of $\mathbb{R}^3$ are rarer compared to such tilings of the plane. For example, there is only a single uniform tiling of $\mathbb{R}^3$ by a regular polyhedron (any of the five Platonic solids), namely, the regular tessellation of cubes. This tiling is uniform with respect to the vertices, edges, and faces of the cubes. The only other known such uniform tiling of $\mathbb{R}^3$ consists of repeat tiling units made up of two regular tetrahedra and one regular octahedron, which is the Delaunay tessellation (17) of the face-centered cubic (fcc) lattice. The latter is the network obtained by inserting "bonds" between nearest-neighbor lattice sites. Until the present work, it was believed that such a tiling, called the "octet truss" by Buckminster Fuller, and its associated stacking variants were the only tessellations of $\mathbb{R}^3$ that involve two different regular polyhedra.

Here we identify and analyze a unique family of periodic tilings of $\mathbb{R}^3$, parameterized by the single scalar $\alpha \in (0,1/3]$, whose smallest repeat tiling unit consists of one regular octahedron and six smaller regular tetrahedra. We first derive an extreme member of this unique family of tilings by showing that the "holes" of the optimal lattice packing of octahedra, which was first discovered by Minkowski over one hundred years ago, are congruent tetrahedra whose edge length is one third of that of the octahedron. We find that this tiling possesses 694 distinct concave (i.e., nonconvex) repeat tiling units, 24 of which are centrally symmetric, and thus is distinctly different and combinatorically much richer than the fcc tetrahedra-octahedra tiling, which only has two distinct tiling units with only one possessing central symmetry. We then construct a one-parameter family of octahedron packings that correspond to a continuous deformation of the fcc lattice

Author contributions: J.H.C., Y.J., and S.T. designed research; J.H.C., Y.J., and S.T. performed research; J.H.C., Y.J., and S.T. contributed new reagents/analytic tools; J.H.C., Y.J., and S.T. analyzed data; and J.H.C., Y.J., and S.T. wrote the paper.

The authors declare no conflict of interest.

*This Direct Submission article had a prearranged editor.

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This article contains supporting information online at www.pnas.org/lookup/suppl/doi:10.1073/pnas.1105594108/-/DCSupplemental.

MATHEMATICS

packing with $\alpha = 0$ that ultimately ends with the optimal lattice packing of octahedra with $\alpha = 1/3$. We find that the holes in these packings, except for the two extreme cases (i.e., $\alpha = 0$ and $1/3$) are tetrahedra of two sizes, leading to periodic tilings having smallest repeat tiling units composed of four small tetrahedra and two large tetrahedra that contact an octahedron, whose structural characteristics are even richer. In particular, the tilings with $\alpha \in (0,1/3)$ possess 2,068 distinct concave repeat tiling units, 62 of which are centrally symmetric. As one transverses the tilings in this family starting from the fcc tetrahedra-octahedra tiling ($\alpha = 0$), the small tetrahedra grow and the large ones shrink until they become equal in size in the tiling associated with the optimal lattice packing of octahedra ($\alpha = 1/3$). These tilings could be used to model complex multicomponent molecular and nano-particle systems and enable one to design building blocks for targeted self-assembly (18, 19).

A New Tiling of $\mathbb{R}^3$ by Tetrahedra and Octahedra Derived from the Optimal Lattice Packing of Octahedra

Recently, an efficient polyhedron packing protocol, called the adaptive-shrinking-cell scheme, was employed to provide strong evidence that the optimal lattice packings of the centrally symmetric Platonic (cube, octahedron, dodecahedron, and icosahedron) and Archimedean solids are the densest packings (20, 21). A polyhedron is centrally symmetric if it contains a point of inversion symmetry. This recent work on polyhedron packings brought attention to a classical century-old result of Minkowski (22) in which the optimal lattice packing of octahedra was first reported. What is remarkable is that in all this time no one seems to have recognized that the holes in the optimal lattice packing of octahedra are equal-sized regular tetrahedra and that one can associate a concave unit consisting of a single octahedron in this packing and a certain subset of six contacting tetrahedra (which fill the holes) that periodically tiles or fills 3D space.

Why did it take so long to make this discovery? First, the lattice associated with the optimal octahedron packing does not possess striking symmetries, such as those possessed by the fcc lattice. Second, studies of particle packings have focused mainly on spherical objects and analysis of the holes in sphere packings has primarily involved characterizing the centroids of the holes, not their shapes. Third, graphical visualizations of the optimal octahedron packing aided in bringing our attention to the intriguing hole structure and geometry. This unique tetrahedron-octahedron tiling and the fact that there are many distinct concave units consisting of a single octahedron and six contacting tetrahedra are some of the central results of this paper.

We begin our analysis by examining the optimal lattice packing of octahedra. An octahedron is defined via the relation

$$P_O = \{\mathbf{x} \in \mathbb{R}^3 : |x_1| + |x_2| + |x_3| \le 1\}. \quad [1]$$

Each lattice site is specified by the lattice vectors $\mathbf{a}_1$, $\mathbf{a}_2$, and $\mathbf{a}_3$ of the optimal lattice packing of octahedra:

$$\mathbf{a}_1 = \left(\frac{2}{3},\frac{2}{3},\frac{2}{3}\right)^T, \qquad \mathbf{a}_2 = \left(-\frac{2}{3},1,\frac{1}{3}\right)^T, \qquad \mathbf{a}_3 = \left(-\frac{1}{3},\frac{1}{3},\frac{4}{3}\right)^T. \quad [2]$$

The optimal lattice packing has a density (fraction of $\mathbb{R}^3$ covered by the nonoverlapping particles) of $\phi = 18/19$ (22). The octahedra make partial face-to-face contact with one another in a complex fashion to form a dense packing with small regular tetrahedral holes. The edge length of a tetrahedron is only one third of that of the octahedron and therefore the ratio of the volume of a single octahedron to that of a tetrahedron is 108. Insertion of tetrahedra of appropriate size into the holes results in the unique tetrahedron-octahedron tiling of $\mathbb{R}^3$, which is illustrated in Fig. 2*A*.

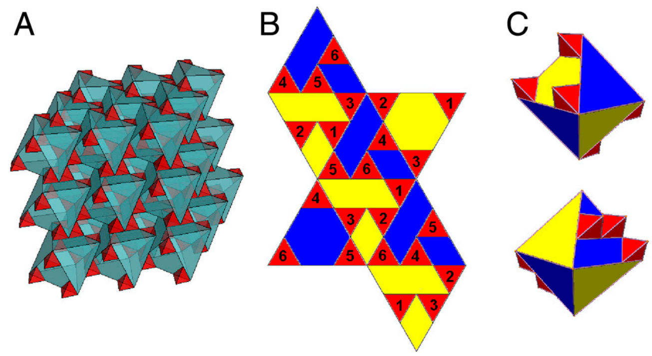

Fig. 2. A new tiling of 3D Euclidean space by regular tetrahedra and octahedra associated with the optimal lattice packing of octahedra. (*A*) A portion of the 3D tiling showing "transparent" octahedra and red tetrahedra. The latter in this tiling are equal-sized. (*B*) A 2D net of the octahedron (obtained by cutting along certain edges and unfolding the faces) with appropriate equal-sized triangular regions for the tetrahedra highlighted. The integers (from 1 to 6) indicate which one of the six tetrahedra the location is associated. Although each octahedron in this tiling makes contact with 24 tetrahedra through these red regions, the smallest repeat tiling unit only contains six tetrahedra, i.e., a tetrahedron can only be placed on one of its four possible locations. The adjacent faces of an octahedron are colored yellow and blue for purposes of clarity. (*C*) Upper box: A centrally symmetric concave tiling unit that also possesses threefold rotational symmetry. Note that the empty locations for tetrahedra highlighted in (*B*) are not shown here. Lower box: Another concave tiling unit that only possesses central symmetry. Observe that the empty locations for tetrahedra highlighted in (*B*) are not shown here.

Fig. 2*B* shows a 2D net of an octahedron (obtained by cutting along certain edges and unfolding the faces) in which the 24 small triangular regions (locations) associated with the tetrahedra are highlighted. A single tetrahedron in this tiling contacts four octahedra. When an octahedron is mapped into a 2D unfolded net, because of the periodicity of the tiling, there are four locations for each of the six tetrahedra in the periodic repeat unit labelled 1, 2, 3, 4, 5, and 6, as shown in Fig. 2*B*. The coordinates of the vertices for the tetrahedra can be written as $(n_1/3, n_2/3, n_3/3)$, where $n_1, n_2, n_3 = 0, \pm 1, \pm 2, \pm 3$. Once a tetrahedron is placed on one of its four possible locations, no tetrahedron can be placed on the remaining three locations. However, each octahedron in this tiling makes contact with 24 small tetrahedra through all of the 24 triangular regions, but this contact configuration is not a repeat unit. The coordinates of the 24 locations are given in the *SI Appendix*.

As can be seen from Fig. 2*B*, because there are many possible ways for placing the six tetrahedra, it is clear that this tiling must have many distinct concave units (i.e., those that are not related by any symmetry operations). A simple counting would lead to $4^6 = 4{,}096$ possibilities, but not all of them are distinct from one another. We explicitly construct all of the 4,096 possible tiling units and find that there only 694 distinct ones, among which 24 possess central symmetry. Fig. 2*C* shows two of the centrally symmetric tiling units and we present all of 694 units in the *SI Appendix*.

FCC Tetrahedra-Octahedra Tiling

It is useful to contrast the aforementioned tetrahedron-octahedron tiling associated with the optimal lattice packing of octahedra with the well known fcc tetrahedron-octahedron tiling or "octet truss." We have noted that the latter tiling can be derived from the fcc lattice packing of octahedra. In particular, consider the octahedron defined by Eq. **1**, which is placed on the lattice sites specified by

$$\mathbf{a}_1 = (1,1,0)^T, \qquad \mathbf{a}_2 = (-1,1,0)^T, \qquad \mathbf{a}_3 = (0,1,1)^T. \quad [3]$$

In this octahedron packing with a density $\phi = 2/3$, four octahedra, each making contacts by sharing edges perfectly with the other three, form a regular-tetrahedron-shaped hole with the same edge length with that of the octahedra. If tetrahedra of proper size are inserted into the holes of the packing, the fcc tetrahedron-octahedron tiling is recovered.

A single tetrahedron in this tiling make perfect face-to-face contact with four octahedra. When an octahedron is mapped into a 2D unfolded net, because of the periodicity of the tiling, there are four locations for each of the two tetrahedra in the periodic repeat unit labelled 1 and 2, as shown in Fig. 3*B*. Due to the central symmetry of an octahedron, this tiling only has two distinct tiling units, as shown in Fig. 3. By placing the tetrahedra on two centrally symmetric faces of the octahedron, one can construct a centrally symmetric rhombohedron that tiles space (upper box of Fig. 3*C*). The coordinates of the vertices for the tetrahedra in this unit are $\{(1,0,0),(1,1,1),(0,1,0),(0,0,1)\}$ and $\{(-1,0,0),(-1,-1,-1),(0,-1,0),(0,0,-1)\}$. The other unit can be obtained by placing a pair of tetrahedra on two adjacent faces of an octahedron, leading to a concave polyhedron with a mirror-image symmetry (lower box of Fig. 3*C*). The coordinates of the vertices for the tetrahedra in this unit are $\{(1,0,0),(1,1,1),(0,1,0),(0,0,1)\}$ and $\{(0,0,1),(0,1,0),(-1,1,1),(-1,0,0)\}$. We note that in this fcc tiling, each octahedron makes perfect face-to-face contacts with eight tetrahedra. It is clear that this tetrahedron-octahedron tiling is considerably structurally simpler than the tiling of $\mathbb{R}^3$ by tetrahedra and octahedra associated with the optimal lattice packing of octahedra reported here.

A Continuous Family of Tetrahedra-Octahedra Tilings

It is noteworthy that the aforementioned fcc packing of octahedra is not "collectively" jammed. Following Torquato and Stillinger (23), a packing is *locally* jammed if no particle in the system can be translated while fixing the positions of all other particles. A *collectively* jammed packing is a locally jammed packing such that no subset of particles can simultaneously be continuously displaced so that its members move out of contact with one another and with the remainder set. A packing is *strictly* jammed if it is collectively jammed and all globally uniform volume nonincreasing deformations of the system boundary are disallowed by the impenetrability constraints. Readers are referred to ref. 23 for further details.

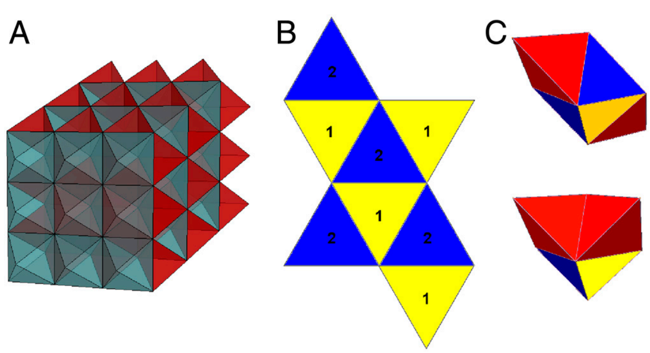

Fig. 3. The well known tiling of 3D Euclidean space by regular tetrahedra and octahedra associated with the fcc lattice (or "octet truss.") (*A*) A portion of the 3D tiling showing "transparent" octahedra and red tetrahedra. (*B*) A 2D net of the octahedron obtained by cutting along certain edges and unfolding the faces. Each octahedron in this tiling makes perfect face-to-face contact with eight tetrahedra whose edge length is same as that of the octahedron. Thus, we do not highlight the contacting regions as in Fig. 2*B*. The integers (1 and 2) on the contacting faces indicate which one of the two tetrahedra the face is associated. As we describe in the text, the smallest repeat unit of this tiling contains two tetrahedra, each can be placed on one of its four possible locations, leading to two distinct repeat tiling units shown in (*C*). The adjacent faces of an octahedron are colored yellow and blue for purposes of clarity. (*C*) Upper box: The centrally symmetric rhombohedral tiling unit. Lower box: The other tiling unit which is concave (nonconvex).

In the fcc packing of octahedra, adjacent square layers of octahedra can slide relative to one another. This fact implies that in general there should be a noncountably infinite number of continuous deformations of the fcc packing that densifies the packing until the densest lattice packing of octahedra is reached. Because both the fcc and optimal lattice packings of octahedra correspond to tetrahedra-octahedra tilings, it is natural to ask whether there exists a very special deformation for which each intermediate packing between the fcc and optimal lattice packing also corresponds to a tetrahedra-octahedra tiling. Indeed, we show below that there is a unique deformation that provides a continuous family of tetrahedra-octahedra tilings.

Consider the following one-parameter family of lattice packings of octahedra with the basis vectors:

$$\begin{aligned} \mathbf{a}_1 &= (1-\alpha, 1-\alpha, 2\alpha)^T, \qquad \mathbf{a}_2 = (-1+\alpha, 1, \alpha)^T, \\ \mathbf{a}_3 &= (-\alpha, 1-2\alpha, 1+\alpha)^T, \end{aligned} \tag{4}$$

where $\alpha \in [0,1/3]$. This one-parameter family provides a continuous set of octahedron packings that span from the fcc packing when $\alpha = 0$ to the optimal lattice packing when $\alpha = 1/3$ and it is constructed by comparing the lattice vectors of the two extreme packings. The packing density ϕ as a function of α is given by

$$\phi = \frac{2}{3}\frac{1}{1-2\alpha+4\alpha^2-2\alpha^3}. \tag{5}$$

When $\alpha = 0$ and $1/3$, one recovers from Eq. **5** $\phi = 2/3$ and $\phi = 18/19$ for the fcc packing and optimal lattice packing, respectively.

As α moves immediately away from zero, each octahedron in the packing makes partial face-to-face contact with 14 neighbors, leading to 24 tetrahedron holes for each octahedron, three on

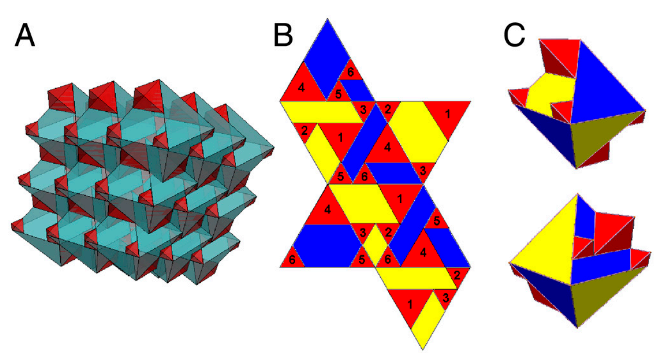

Fig. 4. A member of the continuous family of tetrahedra-octahedra tilings of 3D Euclidean space with $\alpha = 1/4$. (*A*) A portion of the 3D tiling showing "transparent" octahedra and red tetrahedra. (*B*) A 2D net of the octahedron (obtained by cutting along certain edges and unfolding the faces) with appropriate sites for the tetrahedra highlighted. As we describe in the text, the tetrahedra in the tiling are of two sizes, with edge length $\sqrt{2}\alpha$ and $\sqrt{2}(1-2\alpha)$. The integers (from 1 to 6) indicate which one of the six tetrahedra the location is associated. Although each octahedron in this tiling makes contact with 24 tetrahedra through these red regions, the smallest repeat tiling unit only contains six tetrahedra (two large and four small). As α increases from 0 to 1/3, the large tetrahedra shrinks and the small ones grow, until $\alpha = 1/3$ at which the tetrahedra become equal-sized. For $\alpha = 1/4$, the edge length of the large tetrahedra is twice of that of the small ones. The adjacent faces of an octahedron are colored yellow and blue for purposes of clarity. (*C*) Upper box: A centrally symmetric concave tiling unit corresponds to that shown in the upper box of Fig. 2*C* (with $\alpha = 1/3$). Note that the empty locations for tetrahedra highlighted in (*B*) are not shown here. Lower box: Another centrally symmetric concave tiling unit corresponds to that shown in the lower box of Fig. 2*C* (with $\alpha = 1/3$). Observe that the empty locations for tetrahedra highlighted in (*B*) are not shown here.

MATHEMATICS

each faces of the octahedron, with edge length $\sqrt{2}\alpha$, $\sqrt{2}\alpha$, and $\sqrt{2}(1-2\alpha)$ (see Fig. 4). When α is small, one of the three tetrahedra on a triangular face of an octahedron is much larger than the remaining two, almost occupying the entire triangular face. The large tetrahedra with edge length $\sqrt{2}(1-2\alpha)$ correspond to the tetrahedra with edge length $\sqrt{2}$ in the fcc tetrahedra-octahedra tiling (with $\alpha = 0$). Thus, a repeat tiling unit only contains two large tetrahedra, each of which can be placed on one of the four possible triangular regions (locations) on the faces of an octahedron, as in the fcc tetrahedra-octahedra tiling (see Fig. 3*B* and Fig. 4*B*). However, here each tiling unit also contains four additional small tetrahedra with edge length α, each of which can be placed on one of four possible locations (see Fig. 4*B*). Therefore, these tiling units are combinatorically richer than those of the fcc tetrahedra-octahedra tiling and the tiling associated with the optimal lattice packing of octahedra that we discovered here. In particular, any tiling with $\alpha \in (0,1/3)$ (not including the extreme cases) possesses 2,068 distinct concave repeat tiling units, 62 of which have central symmetry. The coordinates of the triangular regions (i.e., the locations of tetrahedra contacting an octahedron) and all of the tiling units are given in the *SI Appendix*.

As α increases from 0 to 1/3, the octahedron packing continuously deforms from the fcc packing to the optimal lattice packing (see the Movie cited in the *SI Appendix*). In the corresponding tilings, the large tetrahedra shrink while the small ones grow until all of the tetrahedra become equal in size in the tiling associated with the optimal lattice packing of octahedra. Thus, we explicitly construct a continuous family of tetrahedra-octahedra tilings that span two aforementioned extremes.

Conclusions and Discussion

We have discovered a unique one-parameter family of periodic tilings of $\mathbb{R}^3$ whose smallest repeat tiling unit consists of one regular octahedron and six smaller regular tetrahedra. We obtained this family of tilings by explicitly constructing a family of octahedron packings that continuously spans from the fcc packing ($\alpha = 0$) to the optimal lattice packing of octahedra ($\alpha = 1/3$) and then showing that the holes are tetrahedra. All members of this family of tilings with $\alpha \in (0,1/3)$ possess 2,068 distinct concave repeat tiling units composed of two large tetrahedra and four small tetrahedra contacting an octahedron, 62 of which are centrally symmetric. In the extreme case of $\alpha = 1/3$, the tiling has 694 distinct concave repeat tiling units composed of six congruent tetrahedra contacting an octahedron, 24 of which possess central symmetry. As one transverses the tilings in the family starting from the well known fcc tetrahedra-octahedra tiling (not a member of the aforementioned tiling family), the small tetrahedra grow and the large ones shrink until they become equal in size in the tiling associated with the optimal lattice packing of octahedra. We also demonstrated that the tilings with α in $(0,1/3)$ are distinctly different and combinatorically richer than the fcc tetrahedra-octahedra tiling ($\alpha = 0$). Note that the principle that packings in $\mathbb{R}^d$ which are not collectively jammed can lead to denser packings by either infinitesimal or finite motions (translations and rotations) of the particles is quite general, applying to packings of particles with arbitrary shape. The class of noncollectively jammed packings in which infinitesimal or continuous motions densify the packings (such as the ones found here) is more restrictive, but includes convex polytopes and hyperspheres, among other objects.

Do tilings similar to the ones reported in this paper exist in other Euclidean space dimensions? In $\mathbb{R}^2$, the analogs of the tetrahedron and octahedron are the equilateral triangle and square, respectively. The closest 2D analog of the fcc tetrahedra-octahedra tiling consists of alternating strips of squares and equilateral triangles, in which each fundamental cell contains one square and two triangles. However, this tiling does not possess square symmetry, nor do the squares touch one another along all lattice vectors, which is to be contrasted with the fcc tetrahedra-octahedra tiling in which octahedra form perfect edge-to-edge contacts with their neighbors. In $\mathbb{R}^4$, the analogs of the tetrahedra and octahedra are 4D regular simplex and orthoplex (or cross-polytope), which are not associated with a tiling of $\mathbb{R}^4$. It is worth noting that the analog of fcc lattice in $\mathbb{R}^4$ is the 4D checker-board lattice D_4, the Delaunay tessellation of which is composed of 4D orthoplices and hemicubes (instead of simplices) (24). We are not aware of any nontrivial analogs of our tetrahedra-octahedra tilings in other dimensions. These observations imply that tiling problems are generally dimension specific and the results for a particular dimension cannot be simply generalized to other dimensions.

ACKNOWLEDGMENTS. This work was supported by the Division of Mathematical Sciences at the National Science Foundation under Award Number DMS-0804431 and by the Materials Research Science and Engineering Center (MRSEC) Program of the National Science Foundation under Award Number DMR-0820341.

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