PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A
MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

Geodesic Domes and Fullerenes [and Discussion]

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Geodesic domes and fullerenes

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The structural form of geodesic domes, composed of pentagons and hexagons, played an important role in understanding the structure of carbon clusters. In this paper an analogy between geodesic domes and fullerenes is investigated. A brief survey is given of the geometry of geodesic domes applied in engineering practice, in particular of the geodesic domes bounded by pentagons and hexagons. A connection is also made between these sorts of geodesic domes and the mathematical problem of the determination of the smallest diameter of n equal circles by which the surface of a sphere can be covered without gaps. It is shown that the conjectured solutions to the sphere-covering problem provide topologically the same configurations as fullerene polyhedra for some values of n. Mechanical models of fullerenes, composed of equal rigid nodes and equal elastic bars are also investigated, and the equilibrium shapes of the space frames that model C_{28}, C_{60} and C_{240} are presented.

1. Introduction

From visual inspection one can easily discover an analogy between the structure of C_{60} and the inner layer of the structure of the great U.S. pavilion of R. B. Fuller at the 1967 Montreal Expo. This analogy and other geodesic structures of Fuller were responsible for the name of C_{60}: Buckminsterfullerene (Kroto *et al.* 1985). This is not the first time that Fuller's geodesic domes have helped researchers to understand the structure of matter. In the early 1960s Fuller's geodesic domes, especially his tensegrity spheres, inspired Caspar & Klug (1962) to develop the principle of quasi-equivalence in virus research.

The aim of this paper is to investigate the analogy between geodesic domes bounded by pentagons and hexagons and fullerenes. It is possible to construct a network of this sort of geodesic dome by covering the sphere with circles (Tarnai & Wenninger 1990; Pavlov 1990). We shall consider the mathematical problem of determining of the smallest diameter of n equal circles by which the surface of a sphere can be covered without gaps, and shall show that the conjectured solutions to the sphere-covering problem provide topologically the same configurations as fullerene polyhedra for some n.

An easy way of visualizing the structure of fullerenes is to make a physical model, for example, to assemble equal angle planar trivalent connectors and equal length plastic tubes. Mechanically, the polyhedron-like structure so obtained can be considered as a space frame with equal rigid nodes and equal elastic bars such that three bars meet and form angles of 120° at each node. The closed net shape arises by deformation of the bars in a state of self-stress. The edges of the polyhedron obtained

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Figure 1. Geodesic dome in the town of Baku, Azerbaidzhian, erected in 1976. (With the kind permission of Dr G. N. Pavlov.)

will be curved, not straight. We have made calculations to determine the equilibrium shape of the space frames modelling C_{28}, C_{60} and C_{240}. The main results are presented below.

2. Geodesic domes and spherical honeycombs

Although, to my knowledge, the first geodesic dome was designed by W. Bauersfeld and was constructed in the early 1920s in Germany, geodesic domes are associated with the name Richard Buckminster Fuller. Fuller called a dome geodesic if the lines on the surface of the sphere producing a three-way grid are geodesics, that is, great circles of the sphere. These can be obtained in the easiest way if equal regular triangulation is made on all faces of an icosahedron, and the resulting network is projected from the centre of the icosahedron onto the surface of its circumsphere. Later the term *geodesic dome* was used for all polyhedral structures resulting from triangulation of the spherical surface having icosahedral symmetry where the edge lengths of the triangles in the network do not differ too much from each other. The U.S. pavilion at the 1967 Montreal Expo is considered as one of the best examples of a geodesic dome, however, it is a geodesic dome only in the latter, more general sense, since the lines producing the triangular subdivision on the bottom part of the spherical surface are not great circles but small circles of the sphere. Over the years numerous triangular subdivision methods have been developed (Tarnai 1987, 1990).

If the subdivision frequency along an edge of the icosahedron is divisible by 3 then it is easy to make a hexagonal geodesic network from a triangular one by removing the edges. In contrast to geodesic domes of a triangular network, however, geodesic domes with hexagonal networks as single-layer bar-and-joint structures are not rigid. In engineering, hexagonal networks can be applied for single-layer space frames with rigid nodes (an example of this as a dome made of 'dog-bone' elements can be seen in Fuller (1969)), or for plate structures (figure 1); or for one of the layers of double-layer grids. Goldberg (1937) introduced a classification for hexagonal tessellations on the surface of an icosahedron, which also incorporated skewed arrangements. These have been used intensively in virus research (Caspar & Klug 1962), and this idea has also appeared in the fullerene field (Klein *et al.* 1986). It is also possible to apply Goldberg's skewed arrangements to geodesic domes (Tarnai 1984,

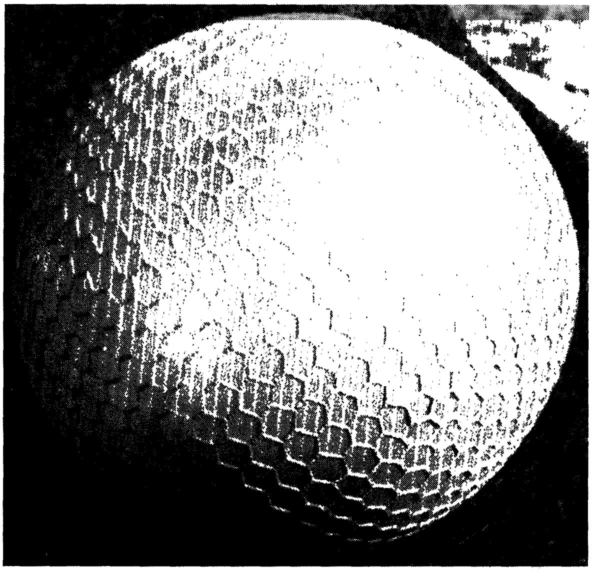

Figure 2. Model of a spherical ‘hexagonal’ net with equal edges and with icosahedral symmetry.

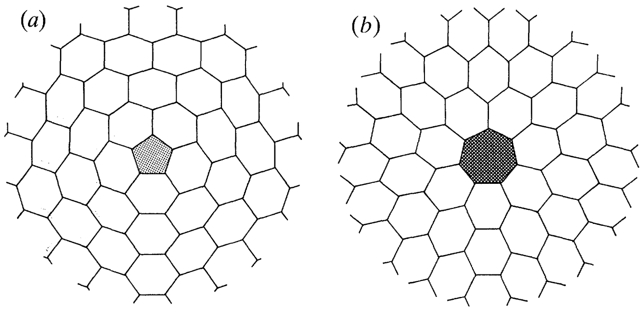

Figure 3. Arrangement of hexagons of equal edge lengths in the plane around an individual (*a*) pentagon with D_5 symmetry and (*b*) heptagon with D_7 symmetry.

1989, Tarnai & Wenninger 1990), but these sorts of domes have not yet been used in practice.

In a triangular subdivision of a spherical surface with icosahedral symmetry – except for the icosahedron itself – the edge lengths in the network are not all equal. A network composed of several hexagons and 12 pentagons can be constructed on the spherical surface with icosahedral symmetry so that the edge lengths are equal (figure 2). In such a network, however, angles of hexagons can differ significantly from the 120° of regular hexagons. In an extreme case, where the common edge length is very small compared with the radius of the sphere, the local spherical networks are approximately planar, and we find that hexagons are elongated in a circumferential direction around the pentagon (figure 3*a*) and that the angles of the hexagons vary between 108° and 144°. If an individual heptagon were to be introduced into a planar ‘hexagonal’ network it would have the opposite effect: the hexagons would be elongated in the radial direction around the heptagon (figure 3*b*) and the angles of the hexagons would vary between 128.6° and 102.8°. If pentagons and heptagons are introduced together, a network can be obtained where the angles

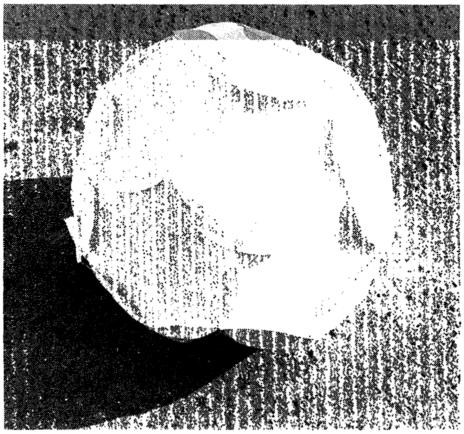

Figure 4. Polyhedron model of locally minimum covering of the sphere by 16 equal circles.

of hexagons remain close to 120°. In nature there are several examples of spherical honeycombs in which some heptagons are involved (Tarnai 1989). Although I do not know of examples of geodesic domes with 5-, 6-, and 7-gonal faces, numerous examples of geodesic domes, especially radomes, exist with triangular network having 5-, 6-, and 7-valent vertices. A remarkable structure can be seen in Schönbach (1971).

The large hypothetical fullerenes are not spherical (Kroto 1988), so it is probably not necessary to have heptagons in the network to keep bond angles close to 120° and thus minimize the potential energy. It is worth mentioning, however, that Mackay & Terrones (1991) suggested a carbon structure fitted to an infinite periodic minimum surface. Because of the negative gaussian curvature of such a surface, it should contain polygons with more than six sides as well as hexagons.

3. Covering the sphere by circles

The different subdivision procedures worked out for the construction of a geodesic dome usually result in distorted hexagons. Pavlov (1990), however, has developed an efficient method for subdividing a spherical surface, which results in inscribed polyhedra (of a sphere) bounded by plane pentagons and hexagons. The geodesic dome in figure 1 was constructed in this way. The circumscribed circles of the polyhedron faces yield an economical way of covering a sphere. Pavlov's method opened up an interesting possibility for building a geodesic dome: to construct a dome with overlapping circles as structural elements (Tarnai & Wenninger 1990).

The problem of how to economically cover a sphere by circles is well known in geometry. In the simplest case, where all the circles are identical, the problem is as follows (Fejes Tóth 1972): how may a sphere be covered by n equal circles (spherical caps) so that the angular radii of the circles are as small as possible? Mathematically proven solutions are known for $n = 2$–7 and for $n = 10$, 12 and 14; conjectured solutions exist for the other values of n up to 20 and for some sporadic values of $n > 20$.

It turns out that there is a correspondence between the topology of arrangements found in the proven and conjectured solutions of the covering problem and various distinct physical problems. Tarnai & Gáspár (1991) analysed the covering problem

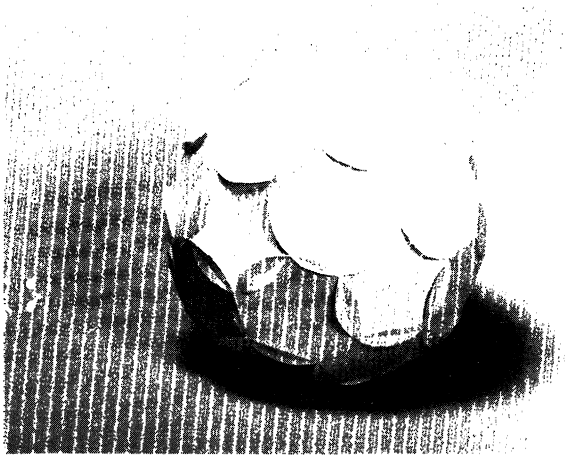

Figure 5. Polyhedron model of locally minimum covering of the sphere by 32 equal circles. (Reprinted from Tarnai & Wenninger (1990) with permission of *Structural Topology* (Montreal) and Dr M. J. Wenniner.)

for small numbers of circles on the basis of the structural form of coated vesicles. Tarnai (1991) pointed out that the coated vesicles identified by Crowther *et al.* (1976) and an additional one having a truncated icosahedron form provide the best covering configurations for $n = 16$, 20 and 32. Interestingly, among the conjectured solutions resulting in local optima, for $n = 16$, 18 and 32 we obtained topologically the same configurations as those of Kroto (1988) published for C_{28}, C_{32}, and C_{60} (Tarnai & Gáspár 1991). The configurations of the conjectured solutions of the covering problem for $n = 16$ and 32 are shown in figures 4 and 5.

Inspection of the structure in figure 5 reveals that the length of an edge separating a pentagon from a hexagon is greater than the length of an edge separating two hexagons. This property of covering the sphere by 32 equal circles (considering only its tendency and not the actual lengths) is consistent with the measurements of C_{60} by Hedberg *et al.* (1991) who found the bond lengths in the five-member rings to be larger than the lengths of bonds fusing the six-membered rings.

4. Stick models of fullerenes

A simple way to appreciate the shape of fullerene is to construct a physical model in which rigid planar trivalent nodal connectors represent the atoms and flexible plastic bars (tubes) of circular cross-section represent the bonds. From a mechanical point of view the model may be considered as a polyhedron-like space frame whose equilibrium shape is due to self-stress caused by deformation of bars. We suppose that the bars are equal and straight in the rest position and that they are inclined relative to each other at every node with angle of 120°. The material of the bars is assumed to be perfectly elastic and that Hooke's law is valid. All the external loads and influences are neglected and only self-stress is taken into account. Then we pose the question: What is the shape of the model subject to these conditions? To answer this question we apply the idea used for coated vesicles by Tarnai & Gáspár (1989).

Let us first investigate this mechanical problem for the model of C_{28} having tetrahedral symmetry (Kroto 1988), and arrange the structural elements in a plane and join the corresponding bar ends and nodes. As a result, a ball-like space frame

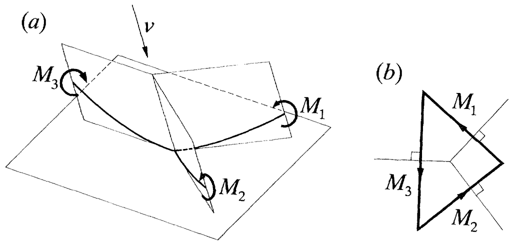

Figure 6. Equilibrium of a node. (*a*) Three bars bending at a node. (*b*) Closed triangle of moment vectors in a plane perpendicular to line v.

is obtained whose bars are no longer straight but curved. Bending the bars generates a state of self-stress in the frame. Due to symmetry, the bars of the frame take on plane-curve form and thus do not twist. This allows us to surmise that the bars of the space frame are under pure bending. The axis of a bar in pure bending takes on the form of a circular arc in the plane of the bend. The bending moments (couples) can be represented by vectors which are perpendicular to the plane of bending.

Let us consider the equilibrium of a node. At a node three bars meet and are subject to bending moments M_1, M_2 and M_3 (figure 6*a*). Under the influence of these moments the bars bend and their axes become circular arcs of radii R_1, R_2 and R_3 respectively, and these circular arcs lie in three different planes. The node is in equilibrium if the vectors of the three bending moments form a closed triangle (figure 6*b*). Since every bending moment vector is perpendicular to its plane, the vector triangle is closed only if the three planes (i.e. the planes of circular arcs) intersect in a common line v. In general, this line v is not perpendicular to the common tangent plane of the curved axes of the three bars at the node, but because of the above-mentioned property, it is perpendicular to the plane of the vector triangle.

The whole space frame is in equilibrium if every node is in equilibrium, i.e. if the bending moment vectors of the bars form a closed polyhedron bounded by triangles. Due to the perpendicularity conditions, the polyhedron formed by the bending moment vectors will be the dual of the curved edge polyhedron. The curved-edged primal polyhedron, i.e. the model itself – due to symmetry – has three different kinds of edges: AB, BC, CC (circular arcs of radii R_1, R_2, R_3) as seen in figure 7*a*, and the dual polyhedron has three different edge lengths: M_1, M_2, M_3 (figure 7*b*). The nodes of the model do not lie on a single spherical surface. In the unit edge length case the radii and the chord lengths of the edges are:

$$R_1 = 1.43760214, \qquad |\mathrm{AB}| = 0.979960623,$$
$$R_2 = 1.62321490, \qquad |\mathrm{BC}| = 0.984261033,$$
$$R_3 = 2.07219822, \qquad |\mathrm{CC}| = 0.990324758.$$

Coordinates of nodes are given in Tarnai & Gáspár (1989).

The C_{60} model has two different kinds of bar forms: AA′ and AA″ (circular arcs of radii R_1 and R_2) as seen in figure 8. In the unit bar length case, the radii and the chord lengths of the curved bar axes are:

$$R_1 = 2.45953818, \qquad |\mathrm{AA'}| = 0.993126401,$$
$$R_2 = 2.31046566, \qquad |\mathrm{AA''}| = 0.992212954.$$

The model looks like a geodesic dome since all the nodes lie on a single sphere whose radius is, interestingly, equal to R_1. Therefore the curved bars which separate two

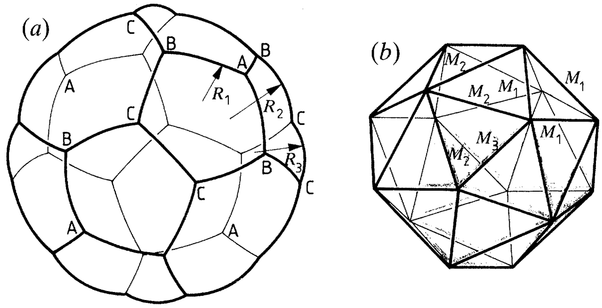

Figure 7. The equilibrium of the space frame modelling C_{28}. (*a*) The primal curved-edged polyhedron formed from bars. (*b*) The dual polyhedron formed from moments.

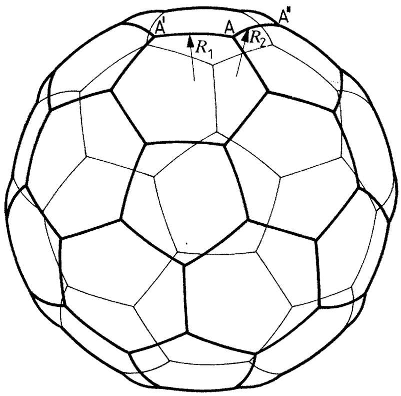

Figure 8. The equilibrium shape of the space frame modelling C_{60}.

adjacent hexagons lie on the same spherical surface. The planes of the curved bars which separate a hexagon and a pentagon do not pass through the centre of the sphere. In this model the chord lengths contrast with the bond lengths measured by Hedberg *et al.* (1991). In the model $|AA'| > |AA''|$, but in C_{60} itself the direction of the inequality is just the opposite: $1.398 < 1.455$.

Kroto & McKay (1988) found that the shapes of stick models of larger icosahedral fullerenes diverge from the geodesic dome form and develop shapes into icosahedral symmetry gradually shifting to the icosahedron as to a polyhedron. Our calculations seem to confirm this trend. The C_{240} model has five different kinds of bar forms. The five bars are shown in a simplified way by thick lines in figure 9 where the large regular triangle composed of dashed lines is a face of the icosahedron. The bars develop pure bending deformations except for bar AC and its symmetric replicas which are also twisted. The unit bar lengths the radii and the chords of the curved bar axes in figure 9 are:

$$R_1 = 2.43731583, \qquad |AB| = 0.993000754,$$
$$R_2 = 2.29406014, \qquad |BB'| = 0.992101446,$$
$$R_3 = 94.3758743, \qquad |CC'| = 0.999995322,$$
$$R_4 = 4.73043037, \qquad |CC''| = 0.998146064,$$
$$|AC| = 0.999523763.$$

The largest deformations occur in the neighbourhood of the vertices of the

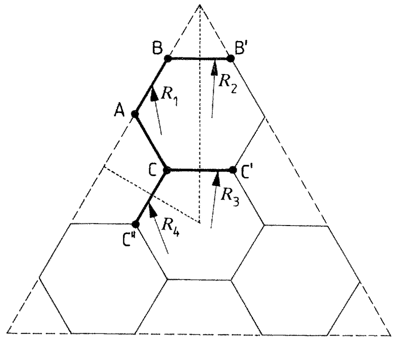

Figure 9. Arrangement of bars of the space frame modelling C_{240} on a face of the icosahedron.

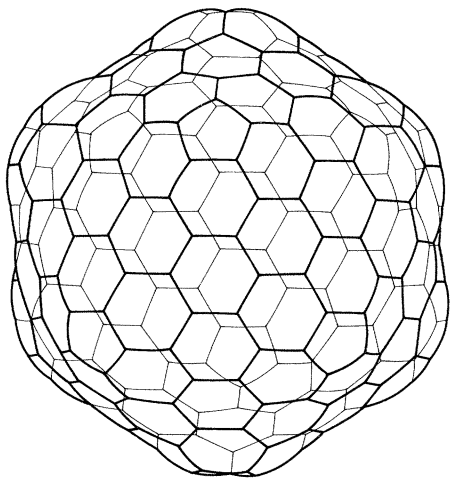

Figure 10. The equilibrium shape of the space frame modelling C_{240}.

icosahedron, and the hexagon in the middle of the faces of the icosahedron becomes flat. For the sake of brevity the coordinates of nodes are not given here; they will be published elsewhere but the complete model is shown in figure 10. Calculations for the model of C_{540} are in progress.

5. Conclusions

The consideration of analogies between geodesic domes and fullerenes is fruitful in both directions. At the very beginning of fullerene research, geodesic dome concepts helped chemists to recognize the structure of these hollow carbon clusters.

In the reverse direction, fullerene studies can indirectly help in the geodesic dome design. The intensive research on fullerenes is providing many suggestions for new structural forms composed of hexagons and pentagons, which may be considered as basic configurations for analysing the fundamental problem of minimum covering of a sphere by circles and also as new configurations for geodesic domes. In this way new geometrical results are also to be expected in the future as a consequence of the detailed studies which are now being carried out on the fullerenes.

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Discussion

S. Iijima (*NEC Corporation, Japan*). I used molecular mechanics to optimize the geometry of giant fullerenes up to C_{960}. Contrary to Professor Kroto's observation, as we optimize the structure approaches a sphere, so the strain is apparently distributed throughout the molecule.

T. Tarnai. A very strong bond deformation should exist in the hexagons of the result is to be spherical.

J. P. Hare (*Sussex University, U.K.*). I have made an icosohedral large fullerene. To make a spherical version of it I have to add heptagon and for every heptagon I must add an extra pentagon. Do you know any simple rules so that I can actually make a large sphere?

P. W. Fowler (*Exeter University, U.K.*). I believe you require 60 heptagons and 60 extra pentagons because they have a plane of symmetry, if you are going icosohedral, and you can do it with a slightly modified spiral algorithm.

T. Tarnai. We don't deal with dynamics; it was a static calculation. We considered elastic bars, which are usually in sub-stress. We found the equilibrium configuration, under which the structure has a certain shape, and in this case we can find only the coordinates of the proper nodes. We found the planes of the curved members which are circular or curved, and whether or not you have twisted or bent elements. In this case the member forms a helix too, but we can make no further comment at this stage.

P. W. Fowler. I was thinking of the actual moment from your initial guess as to the structure towards your bent and bulging final structure. So it is a process in time, but not actually dynamic. Furthermore, there is a chemical corollary of this description of the domes, and the rigidity of a structure with triangles, and that is that there is an extention to Euler's theorem using symmetry. This says that the symmetry spanned by the internal coordinates of a deltahedron is the same as the symmetry spanned by the edges. What this means is that any deltahedron skeleton cannot vibrate if it has perfectly rigid bonds. There are no true bending vibrations in deltahedrons, so there is a kind of chemical equivalent to your description.

T. Tarnai. So what can I say about a triangulated sphere is that for a long time mathematicians believed that there was no such structure which had free motion which would constitute a mechanism. One of them proved that such polyhedra do not exist, but Bill Conolly (late 1970s) produced a triangulated sphere which has free motion. This meant that it had a mechanism involving finite motion so if you wish to consider it as a structure that can vibrate, it has motion that causes no stress. Such a structure exists. Later a German mathematician produced another, so we have some examples.

PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A

igure 1. Geodesic dome in the town of Baku, Azerbaidzhian, erected in 1976. (With the kind permission of Dr G. N. Pavlov.)

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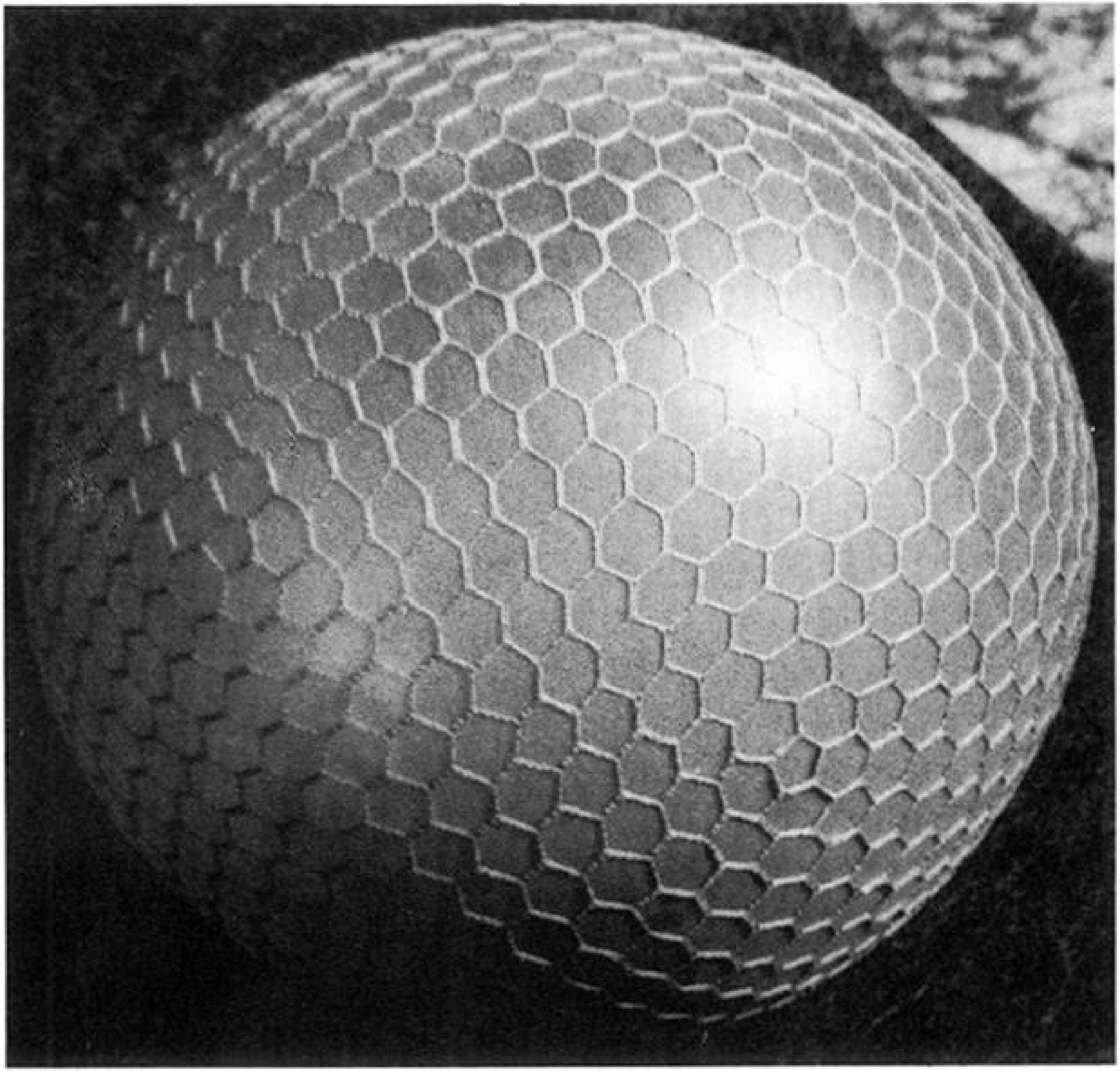
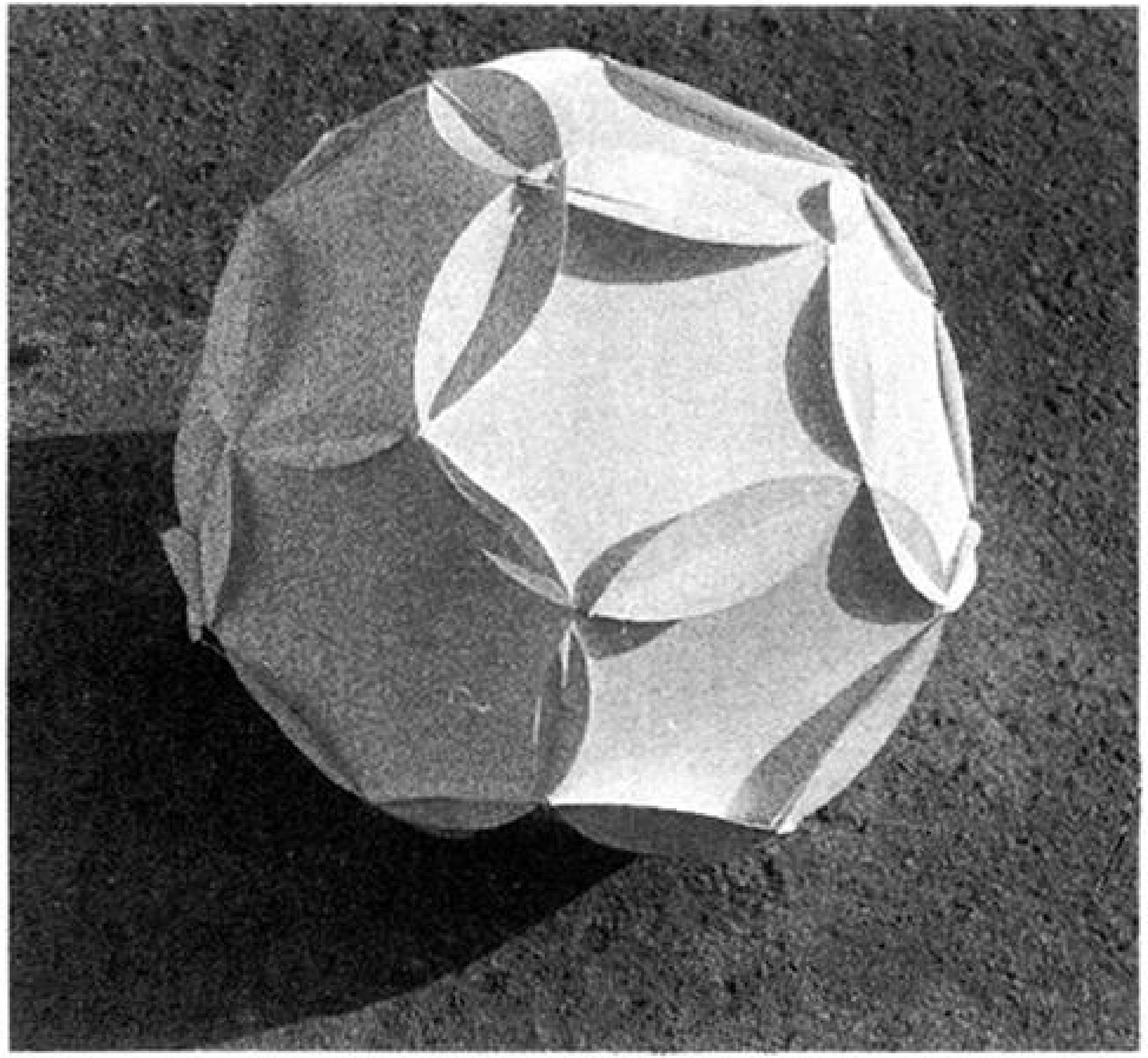
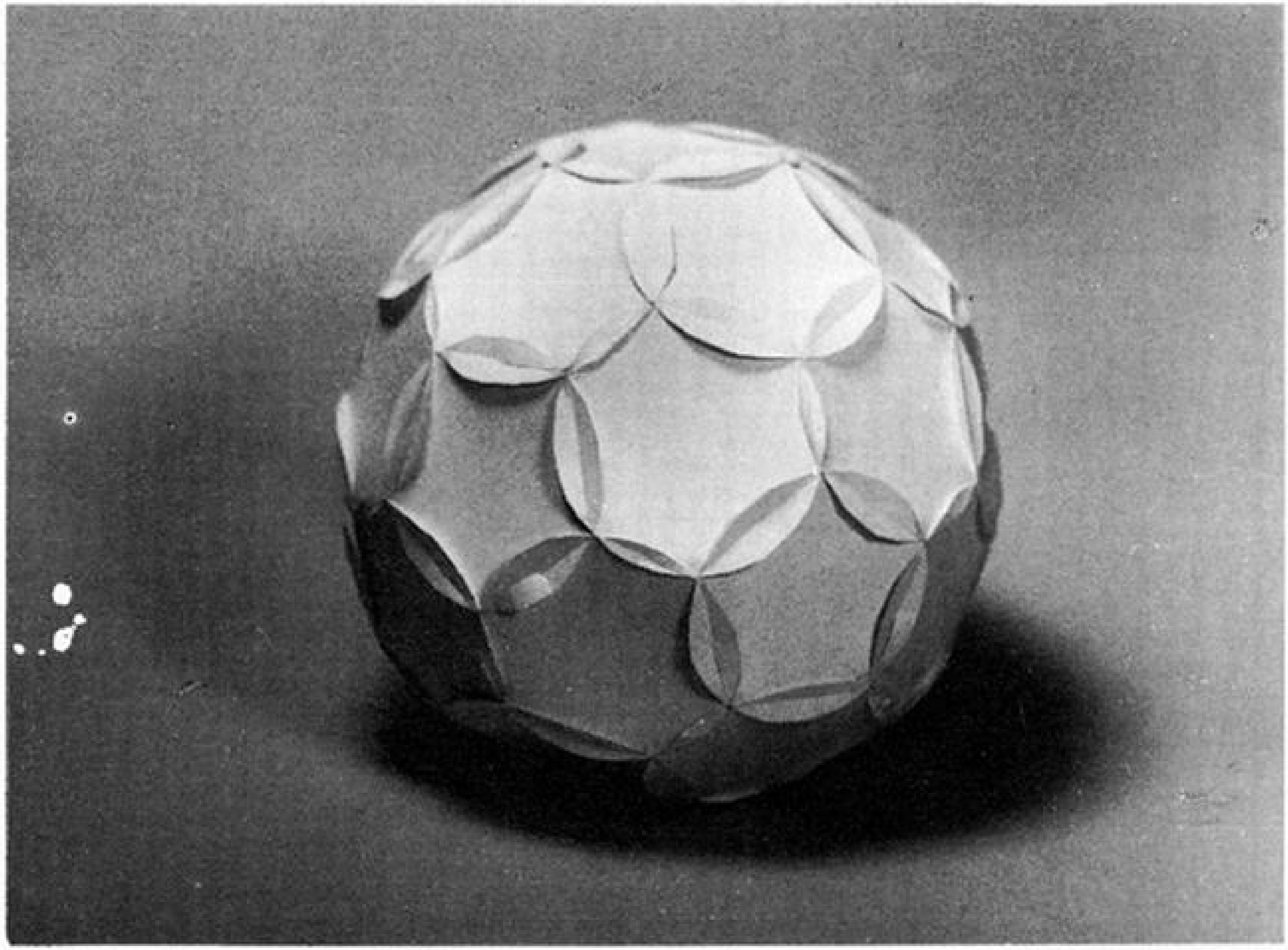


igure 2. Model of a spherical 'hexagonal' net with equal edges and with icosahedral symmetry.



igure 4. Polyhedron model of locally minimum covering of the sphere by 16 equal circles.



igure 5. Polyhedron model of locally minimum covering of the sphere by 32 equal circles. Reprinted from Tarnai & Wenninger (1990) with permission of *Structural Topology* (Montreal) and r M. J. Wenniner.)

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