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Curved graphite and its mathematical transformations

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Mathematical transformations for graphite with positive, negative and zero Gaussian curvatures are presented. When the Gaussian curvature K is zero, we analyse a bending transformation from a planar sheet into a cone. The Bonnet, the Goursat and a mixed transformation are studied for graphitic structures with the same topologies as triply periodic minimal surfaces ($K < 0$). We have found that using the Kenmotsu equations for surfaces of constant mean curvature it is possible to invert spherical and cylindrical graphite. A bending transformation for surfaces of revolution is also studied; during this transformation the helical arrangement of cylinders changes. All these transformations can give an insight into kinematic processes of curved graphite and into new shapes.

1. Introduction

The discovery of C_{60} has opened the field of structures with different curvatures [17,18,20]. In C_{60} and other Fullerenes the Gaussian curvature K (the product of the two principal curvatures, $K = k_1k_2$) is positive, in cylindrical and ordinary graphite K is zero. Structures in which $K < 0$ have been proposed by Mackay and Terrones [24], Lenosky et al. [21], Vanderbilt and Tersoff [36] and O'Keeffe et al. [26]. In this paper we study some mathematical transformations applied to graphitic sheets involving cases where $K = 0, K > 0$ and $K < 0$, so we are not just restricted to a single planar layer of graphite. For surfaces of constant mean curvature like the sphere and the cylinder we have found an interesting transformation which inverts these surfaces; meaning to put the inside of the surface outside and vice versa. This transformation might give an insight in real changes like, for example, in the flipping of corannulene $C_{20}H_{10}$ [29,3,5]. Regarding the plane, a transformation into conical graphite is studied. For the case $K < 0$, we analyse the Bonnet transformation, the Goursat transformation and a mixture of these two. Finally, transformations for helicoidal tubules and spheres are discussed.

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2. Transformation of ordinary graphite into graphitic cones: $K = 0$

Ordinary graphite is made of planar sheets separated by certain distance, so the Gaussian curvature K is zero. If these sheets are rolled up, then cylinders can be obtained; here K is also zero, although one principal curvature has a constant value, therefore, the mean curvature ($H = (k_1 + k_2)/2$) is also constant. Ijima [12] has obtained tubes of graphite which resemble bent graphite sheets. A transformation of a plane into a cylinder has been studied by mathematicians since long time ago and now can have application in the study of graphitic structures. If we take a sheet of paper and bend it to get a cylinder, the distance between two points on the sheet of paper does not change by the process; in fact, this transformation is locally isometric [4,30,31]. Another interesting transformation of a plane consists in changing a planar surface into a cone. This transformation is isometric and can be expressed as follows:

$$x = r \sin\alpha \cos\left[\frac{\theta}{\sin\alpha}\right],$$
$$y = r \sin\alpha \sin\left[\frac{\theta}{\sin\alpha}\right],$$
$$z = r\cos\alpha\,, \tag{1}$$

where $0<\alpha\leqslant\pi/2$ and $0\leqslant\theta\leqslant 2\pi\sin\alpha$. When $\alpha=\pi/2$ a plane is obtained, but when α decreases, conical surfaces are generated (see figs. 1 and 2). During this

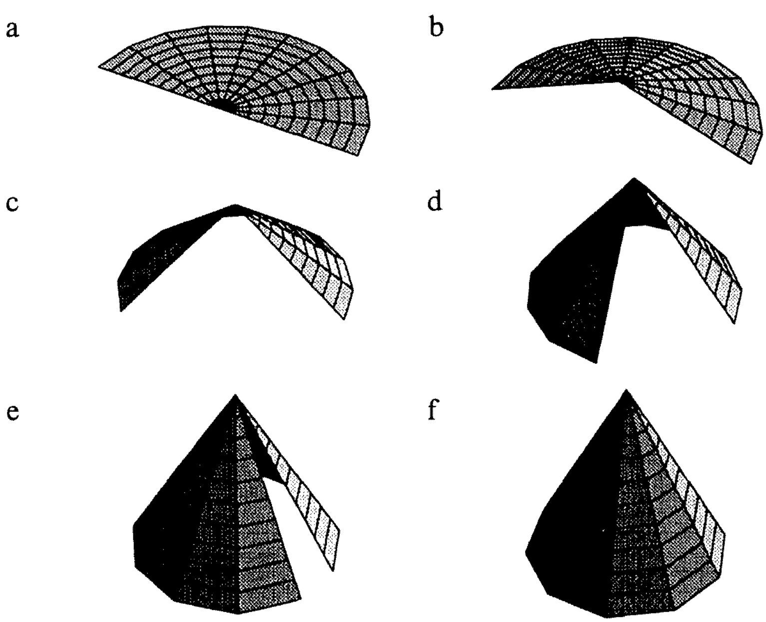


Fig. 1. Transformation of a planar sheet into a cone. (a) $\alpha = \pi/2$. (b) $\alpha = \pi/2.5$. (c) $\alpha = \pi/3.5$. (d) $\alpha = \pi/4.5$. (e) $\alpha = \pi/5.5$. (f) $\alpha = \pi/6$.

a

b

c

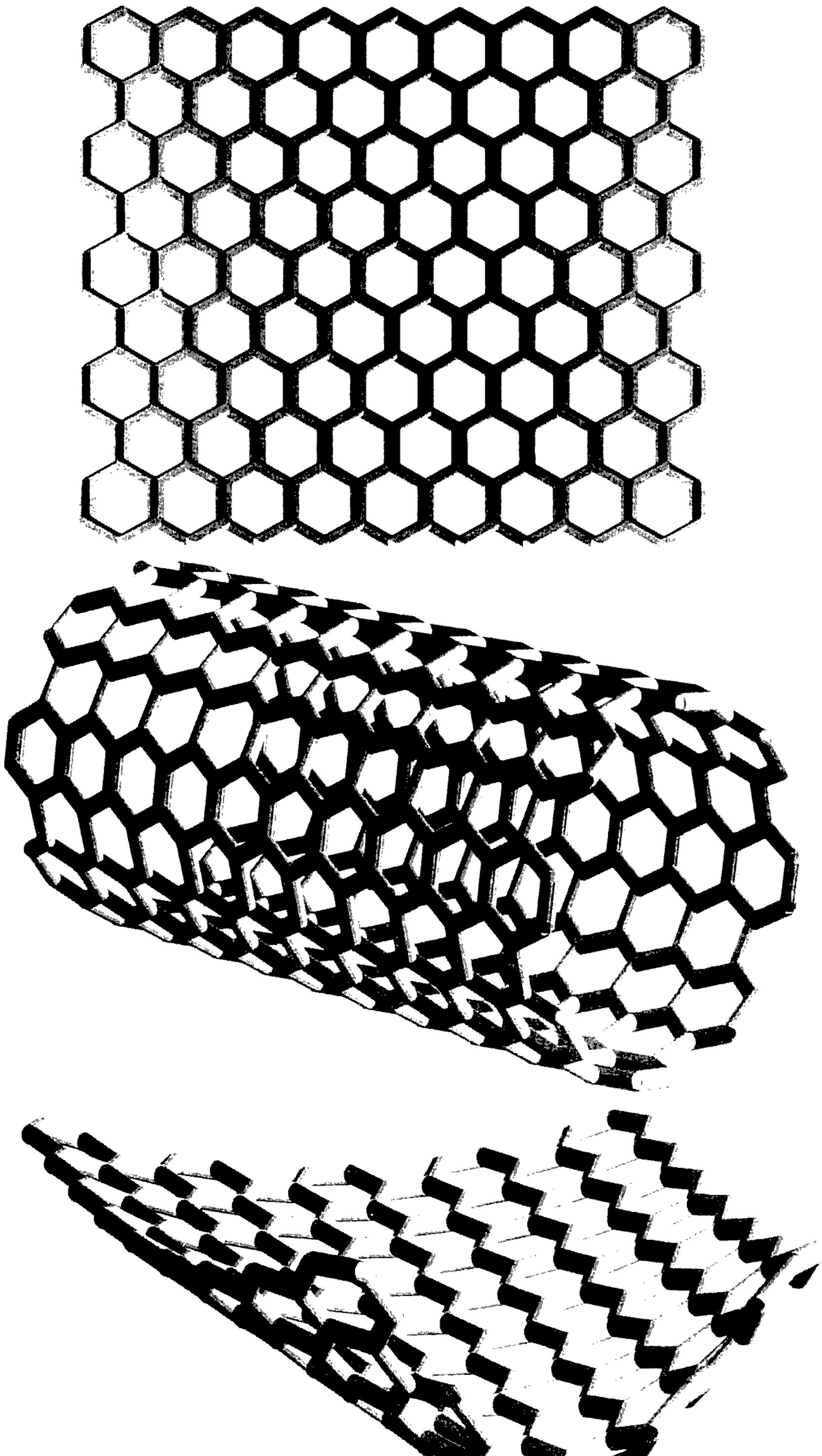


Fig. 2. Different kinds of graphite nets with zero Gaussian curvature ($K = 0$). (a) Ordinary graphite (a plane). (b) Cylindrical graphite. (c) Intermediate state of a transformation for conical graphite.

transformation the metric and the Gaussian curvature remain unchanged, except at the tip of the cone, and can be written as

$$g_{11} = \frac{\partial \boldsymbol{r}}{\partial r} \cdot \frac{\partial \boldsymbol{r}}{\partial r} = 1\,,$$
$$g_{12} = \frac{\partial \boldsymbol{r}}{\partial r} \cdot \frac{\partial \boldsymbol{r}}{\partial \theta} = 0\,,$$
$$g_{22} = \frac{\partial \boldsymbol{r}}{\partial \theta} \cdot \frac{\partial \boldsymbol{r}}{\partial \theta} = r^2\,,$$
$$K = k_1 k_2 = (0)\left(\frac{\cot\alpha}{r}\right) = 0\,,$$
$$H = \frac{\cot\alpha}{2r}\,,$$

where $\boldsymbol{r} = (x, y, z)$, k_1 and k_2 are the principal curvatures, K is the Gaussian curvature and H is the mean curvature. Note that there is a singular point when $\alpha = 0$.

Iijima [13] has also found graphitic cones which are connected to cylinders by a region of negative Gaussian curvature.

3. Transformations for $K < 0$

Negatively curved graphite with topologies similar to triply periodic minimal surfaces (TPMS) is obtained by the introduction of rings with more than six atoms [21,24,26,33,36]. If octagonal rings are used, the exact D, G and P TPMS can be decorated with graphite, so the mean curvature is zero at every point [24,25,28,33,34]. The D, G and P TPMS are related by a transformation discovered by Bonnet last century [2,10,11,27]. The Bonnet transformation preserves the metric, the Gaussian and the mean curvatures, so the surface is just bent without stretching; the classical example of this is the change of a catenoid into a helicoid. For decorating exact TPMS we can use the Weierstrass representation which ensures that the surface obtained is a minimal surface [32–34,37]. The coordinates (x, y, z) in real space of a minimal surface and its Bonnet associated surfaces are given by

$$x = \mathrm{Re}\left[\mathrm{e}^{\mathrm{i}\beta} \int_0^{\omega_0} (1-\omega^2) R(\omega)\,\mathrm{d}\omega\right],$$
$$y = \mathrm{Re}\left[\mathrm{e}^{\mathrm{i}\beta} \int_0^{\omega_0} i(1+\omega^2) R(\omega)\,\mathrm{d}\omega\right],$$
$$z = \mathrm{Re}\left[\mathrm{e}^{\mathrm{i}\beta} \int_0^{\omega_0} 2\omega R(\omega)\,\mathrm{d}\omega\right], \tag{2}$$

where $R(\omega)$ is the Weierstrass function which characterizes each surface. For the D or F surface $R(\omega) = \nu/\sqrt{\omega^8 - 14\omega^4 + 1}$, the values of ω_0 are the points inside the region outlined by the intersection of four circles of radius $\sqrt{2}$ and centres at $(\pm 1/\sqrt{2}, \pm 1/\sqrt{2})$ and ν is a normalization constant, which for C–C in graphite is 7.146 Å. Having the coordinates of a patch in real space, symmetry operations can be used to get an extended part of the surface.

For different values of β, different patches with zero mean curvature can be produced. If $\beta = 0$ a D patch is obtained, when $\beta = 38.0147°$ we get a G patch and with $\beta = \pi/2$ the P patch is generated. All other values of β give patches which cannot be put together without having self intersections and gaps, therefore, just for the three cases mentioned above TPMS can be built. It is interesting to note that the trajectory of points during the Bonnet transformation follow elliptical paths [11]. Figure 3 shows portions of the D, G and P surfaces decorated with graphite.

Another transformation which can be applied to minimal surfaces is the Goursat transformation which stretches and bends the surface [1,7,8]. The coordinates of a Goursat transformed surface are given by

a

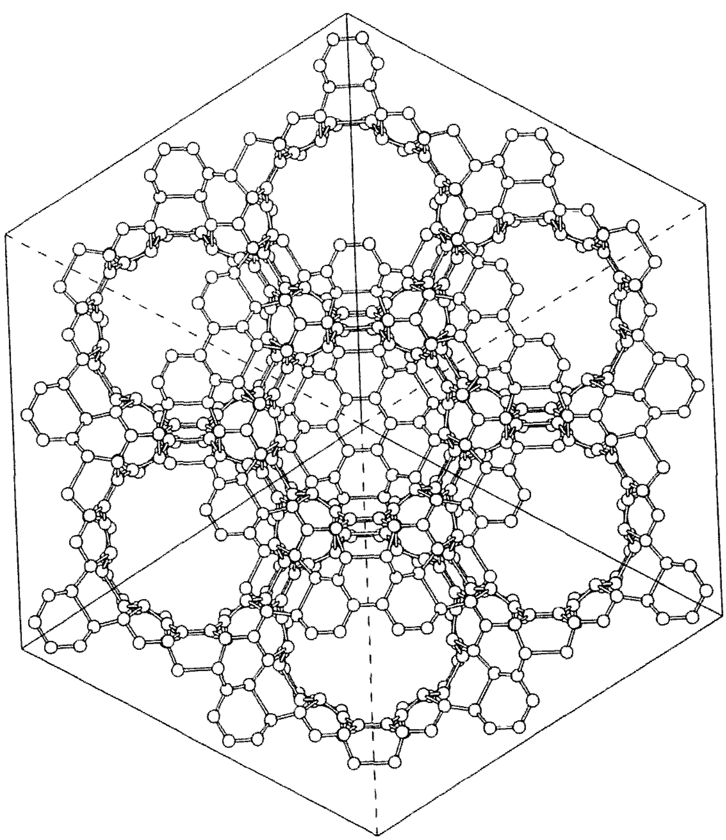
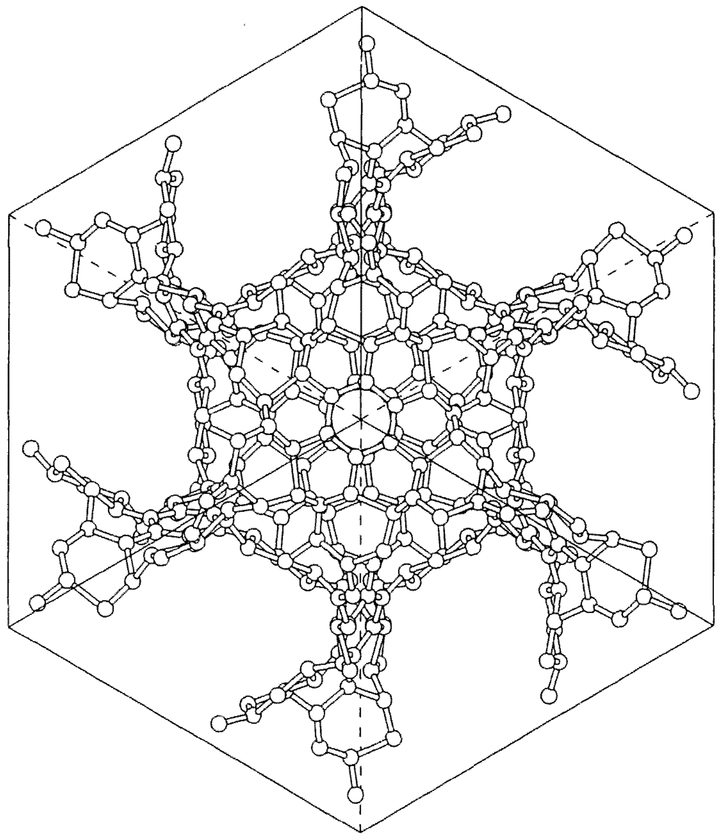


Fig. 3 (continued on next page).

b



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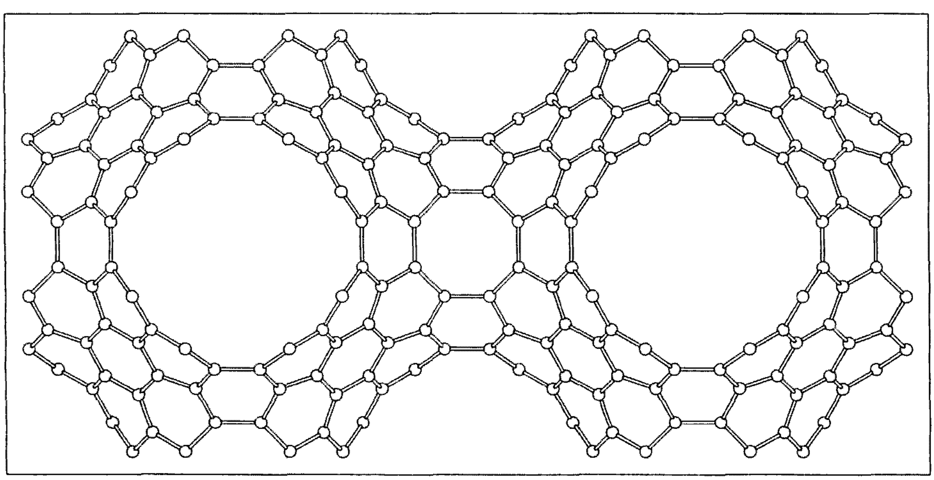

Fig. 3. Negatively curved graphite with octagonal rings and hexagons. (a) Cubic cell of the D surface. (b) Cubic cell of the G surface. (c) Two cubic cells of the P surface.

$$x_G = \mathrm{Re} \int_0^{\omega} R(\omega)\left(k_G - \frac{\omega^2}{k_G}\right) \mathrm{d}\omega\,,$$
$$y_G = \mathrm{Re} \int_0^{\omega} \mathrm{i}R(\omega)\left(k_G + \frac{\omega^2}{k_G}\right) \mathrm{d}\omega\,,$$
$$z_G = \mathrm{Re} \int_0^{\omega} 2R(\omega)\omega \,\mathrm{d}\omega\,, \tag{3}$$

as the value of k_G increases, the surface gets stretched and flatter. Applying the Goursat transformation to a patch decorated with graphite increases the distance among the atoms as the patch is stretched and the atoms get free. Therefore, this transformation is not suitable for structures in which atoms have to stay within a certain range (bond distance). However, it is possible to combine the Bonnet and Goursat transformations and stretch the surface to a small level keeping the structure [33,35]. For this mixed transformation we define $R(\omega)^{\dagger} = R(\omega)\mathrm{e}^{\mathrm{i}\beta}$ and $k_G = 2 - \cos\beta$ or $k_G = 2 - \sin\beta$ in the eq. (3).

4. Transformations for $K \geqslant 0$ and $H = \mathrm{C}$: Spheres and Cylinders

Kenmotsu [15] and Gacksatter [6] have found equations analogous to the Weierstrass equations, but for surfaces with constant mean curvature H. The sphere and the cylinder belong to this kind of surfaces. By introducing a factor $\mathrm{e}^{\mathrm{i}\beta}$ in the Kenmotsu equations we have found a Bonnet-like transformation in which stretching and bending take place; according to this, the Kenmotsu equations can be written as [33]

$$x = -\mathrm{Re}\left[\mathrm{e}^{\mathrm{i}\beta} \int (1 - G^2)\frac{2G^*_{\omega}}{H(1+|G|^2)^2}\,\mathrm{d}\omega\right],$$
$$y = -\mathrm{Re}\left[\mathrm{e}^{\mathrm{i}\beta} \int i(1 + G^2)\frac{2G^*_{\omega}}{H(1+|G|^2)^2}\,\mathrm{d}\omega\right],$$
$$z = -\mathrm{Re}\left[\mathrm{e}^{\mathrm{i}\beta} \int \frac{4GG^*_{\omega}}{H(1+|G|^2)^2}\,\mathrm{d}\omega\right], \tag{4}$$

where $G^*_{\omega} = \frac{1}{2}[\partial G^*/\partial u - \mathrm{i}\partial G^*/\partial v], H$ is the mean curvature and the asterisk denotes the conjugate of a complex variable $(\omega = u + \mathrm{i}v, \omega^* = u - \mathrm{i}v)$. For a unit sphere $G = \omega^*/2$ and $H = 1$. For a unit circular cylinder $G = -(\cos u + \mathrm{i}\sin u)$, $\omega = u + \mathrm{i}v$ and $H = \frac{1}{2}$. An interesting feature of this transformation is that the sphere and the cylinder can be inverted this means to put the inside out and the outside inside (see figs. 4 and 5).

As in the Weierstrass representation, the Kenmotsu equations involve a series of mappings for getting the coordinates in real space. First we go from the complex plane to the Gauss map by stereographic projection and then, from the Gauss map to the surface. The Gauss map or spherical projection consists in the directions

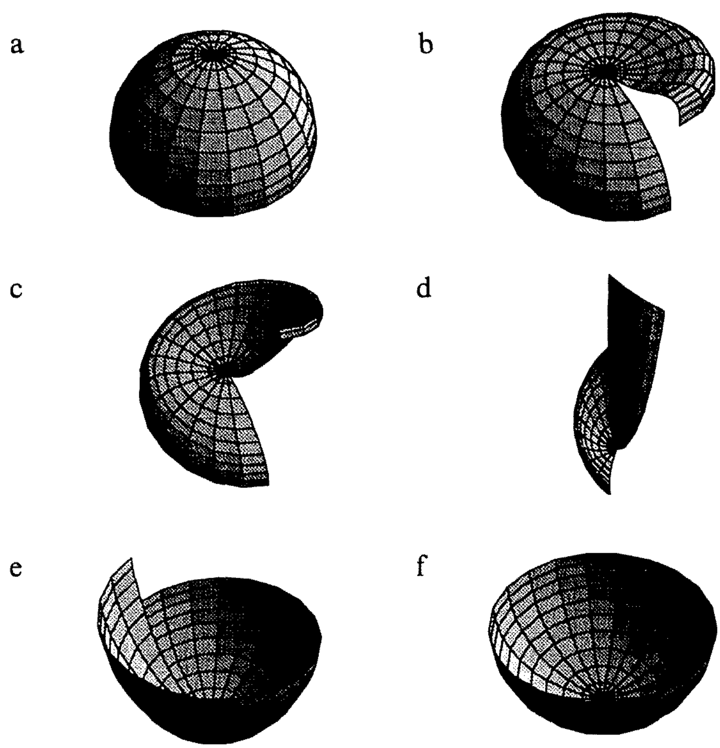

Fig. 4. Inversion of a sphere using Kenmotsu equations for surfaces of constant mean curvature. (a) $\beta = 0$. (b) $\beta = 10°$. (c) $\beta = 20°$. (d) $\beta = 60°$. (e) $\beta = 175°$. (f) $\beta = 180°$.

of the normals to the surface mapped onto a unit sphere [4,30,31]. Summarizing, the series of mappings goes as follows:

Complex plane $\rightarrow$ Stereographic projection $\rightarrow$ Gauss map $\rightarrow$ Surface (x, y, z).

Going from the Gauss map to the complex plane there is just one point that cannot be mapped and this is the north pole. However, since we are dealing with a discrete array of points (atoms) and not with a continuum, this difficulty can be avoided by not choosing an orientation in which one point coincides with the north pole.

In order to perform the transformation we have to start from the complex plane, so the Gauss map for example, of C_{60} or corannulene, has to be projected onto the complex plane to get the coordinates $u + iv$ (see fig. 6). The transformation operating on a sphere and a cylinder are shown in figs. 4 and 5.

A sphere can be decorated with C_{60} or approximate form of other Fullerenes, and also a cylinder can be decorated with graphite to get bucky tubes, therefore, since these structures have constant H, the transformation mentioned above can be carried out. During intermediate states of the transformation stretching takes place, so the structure is unstable, but when $\beta = 0$ and $\beta = \pi$ structures with the

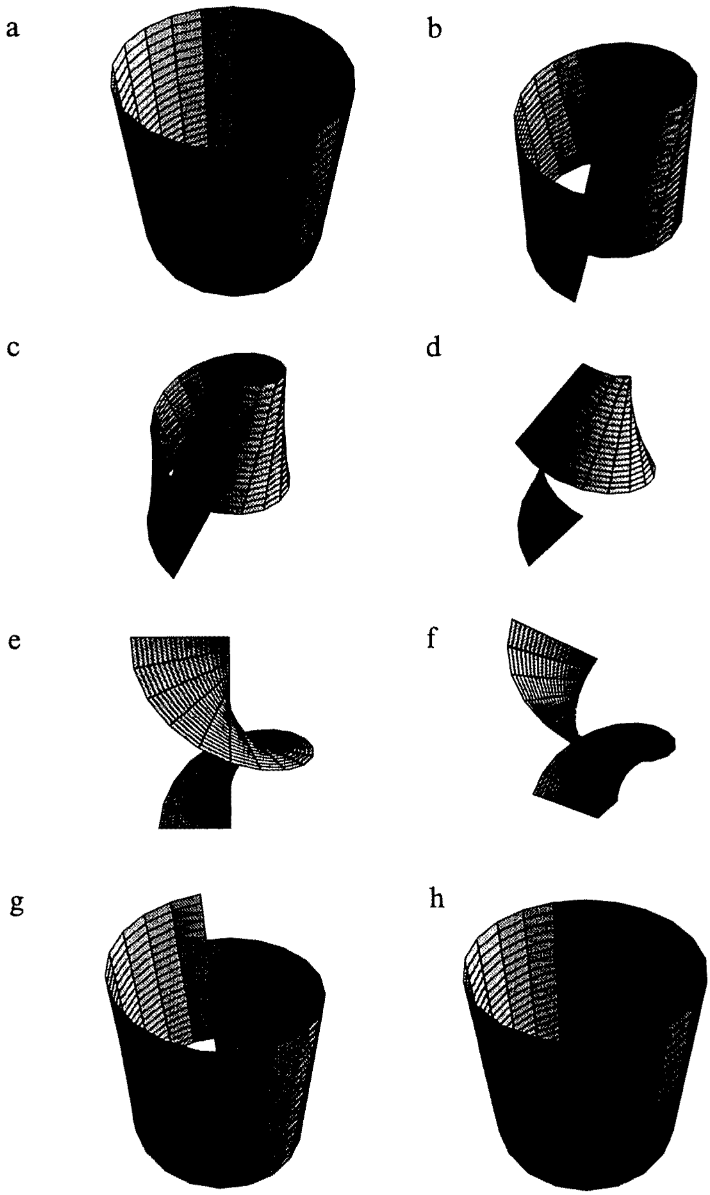

Fig. 5. Inversion of a cylinder using Kenmotsu equations for surfaces of constant mean curvature. (a) $\beta = 0$. (b) $\beta = 10°$. (c) $\beta = 20°$. (d) $\beta = 35°$. (e) $\beta = 90°$. (f) $\beta = 120°$. (g) $\beta = 175°$. (h) $\beta = 180°$.

same bond distances and same angular distributions are generated, although, the structures are inverted. It has been found that corannulene $C_{20}H_{10}$ invertes itself about 2000 times a second [3,29]. A intermediate state which is completely flat has been proposed, here, we offer another possibility by the transformation on surfaces of constant mean curvature.

a

b

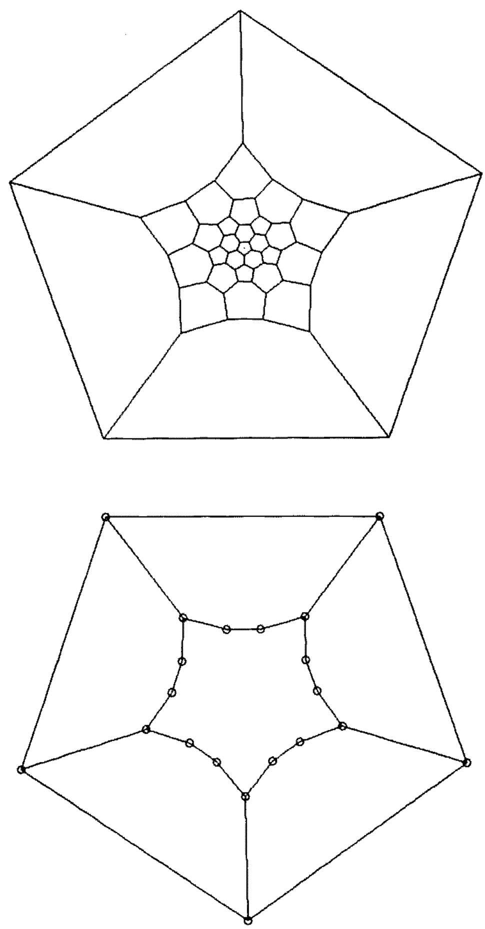

Fig. 6. Stereographic projection on the complex plane: (a) Buckminster-fullerene C_{60}. (b) Corannulene $C_{20}H_{10}$.

5. Transformation for surfaces of revolution

The sphere and the cylinder can be generated by rotating a circular arc and a straight line, respectively, about an axis. Surfaces obtained in this way are called surfaces of revolution; the catenoid, and the cone belong to this family of surfaces. An important result obtained by Boer [16] says that any surface of revolution can be bent. Bearing in mind that spheres and cylinders can be decorated with graphite, we should be able to follow a bending transformation for these structures. The transformation that we are considering consists in rotating and displacing the surface, so we get helicoidal surfaces. For a sphere the transformation takes the following form:

$$x = \rho \cos\theta \sin\alpha\,,$$
$$y = \rho \cos\theta \cos\alpha\,,$$
$$z = \rho \sin\theta + k\alpha\,, \tag{5}$$

where ρ is the radius of the semicircle which corresponds to the radius of the sphere when $k = 0$, θ is the angle which generates the semicircle, α is the angle about which the semicircle is rotated and k is a parameter related to the pitch of the helix. We have chosen a sphere of unit radius for different values of k. When $k = 0$ a perfect sphere is obtained, as k increases, the surface starts to bend in a helical way (see fig. 7). This transformation under the sphere it is not isometric, so the Gaussian curvature changes. The Gaussian curvature can be written as

$$K = [-3k^2 + 3\rho^2 + 4k^2\cos(2\theta) + 4\rho^2\cos(2\theta) - k^2\cos(4\theta) + \rho^2\cos(4\theta)] / [2(k^2 + \rho^2 - k^2\cos(2\theta) + \rho^2\cos(2\theta))^2]\,; \tag{6}$$

as k increases the Gaussian curvature becomes negative close to the borders, however, for small values of k most of the points have positive Gaussian curvature.

In the case of the cylinder the transformation takes the form

$$x = \rho \sin\theta\,,$$
$$y = \rho \cos\theta\,,$$
$$z = v + k\alpha\,, \tag{7}$$

where ρ is the radius of the cylinder, v is a parameter which controls the length of

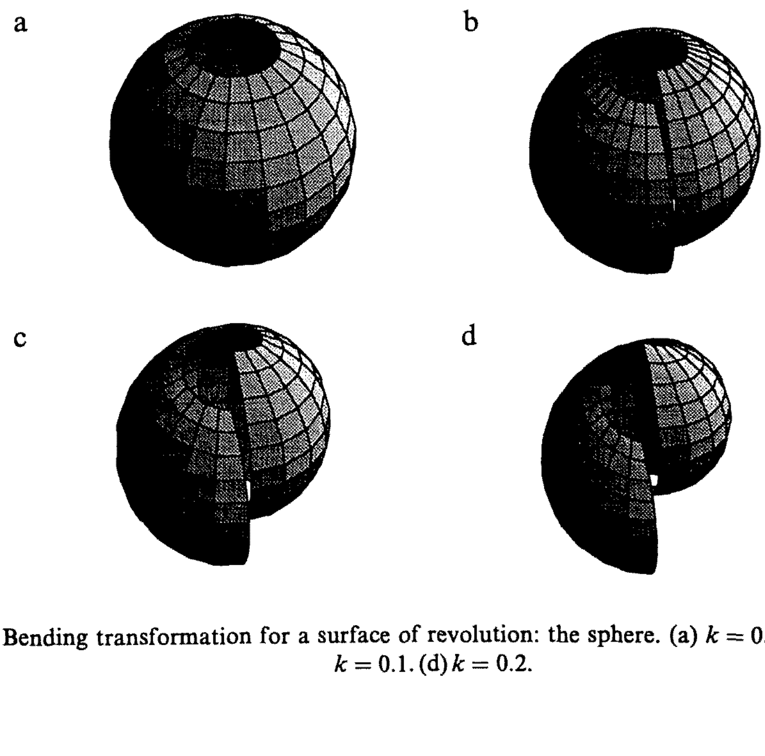

Fig. 7. Bending transformation for a surface of revolution: the sphere. (a) $k = 0$. (b) $k = 0.05$. (c) $k = 0.1$. (d) $k = 0.2$.

the cylinder, α is the rotation angle around the axis of the cylinder and k is a free parameter which involves the pitch of the helix.

For $k = 0$, a perfect cylinder is obtained, as k varies different helicoidal tubules with different degrees of helicity are generated (see fig. 8). Hamada et al. [9] have predicted that the conductivity of cylindrical graphite depends on the diameter of the tubes and on the degree of helical arrangement. According to this, the transformation changes the conductivity of the cylinders. Another important factor here is that the Gaussian curvature remains zero.

Until now helicoidal graphite has not been reported, but it also seems to have an interesting shape. If we look carefully at the Bonnet and the transformations mentioned above, we found that helicoidal states are present in great part of the transformations; further, parallel surfaces can be generated, so several layers might be obtained and transformed [33].

6. Conclusion

Mathematical transformations for the three cases of Gaussian curvatures $K > 0, K = 0$ and $K < 0$ have been studied considering graphite sheets. Among the different shapes of curved graphite we have been able to generate cones, cylinders,

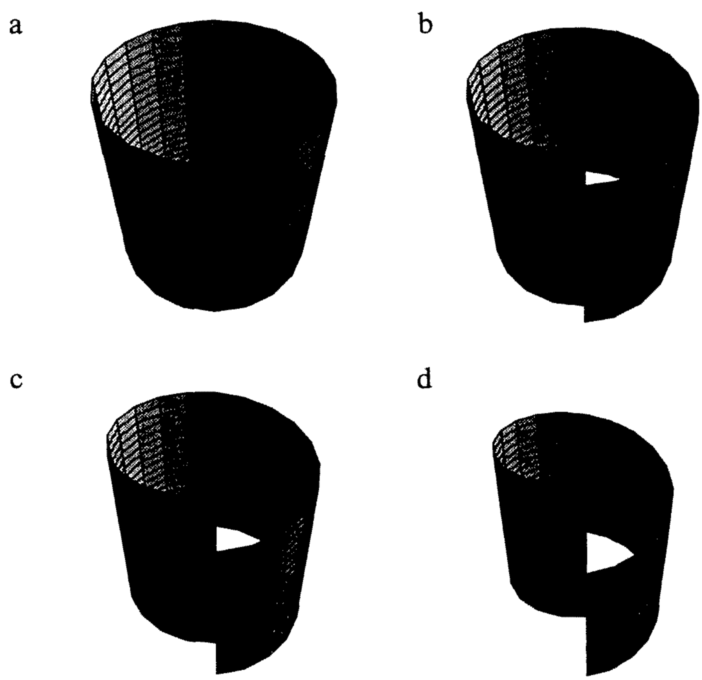

Fig. 8. Bending transformation for a surface of revolution: The cylinder. (a) $k = 0$. (b) $k = 0.05$. (c) $k = 0.1$. (d) $k = 0.2$.

Fullerenes, helicoids and triply periodic minimal surfaces. For surfaces with constant mean curvature a new transformation which uses Kenmotsu equations is introduced. This transformation inverts the sphere and the cylinder and gives another possibility for the flipping of corannulene. The Bonnet and Goursat transformations are also considered; the Goursat transformation is not suitable for structures since its stretching produces atoms to be disconnected. However, a mixed transformation with Bonnet and Goursat terms can stretch and bend the surface to a small degree, so atomic distances are not large, preserving, therefore, the structure. Finally, a transformation for surfaces of revolution is studied; here we find that the transformation when operating on cylinders preserves the Gaussian curvature and cylinders with different degrees of helical arrangement can be obtained.

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