Crystal structures built from highly symmetrical units

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Abstract. — Condensed matter physicists have recently recognised that systems as different as metal elements and metallic alloys with dense atomic packings, semiconductors with covalent tetracoordinated bonds, water clathrates with hydrogen bonds, liquid crystals of cholesteric molecules with double twist and liquid crystals of amphiphilic molecules at liquid/liquid interfaces, build crystal structures exhibiting particular characteristics : namely cubic symmetries with no directly apparent relation to local order and cell parameters much larger than the typical interaction distances. Indeed it appears that the local order cannot propagate over long distances in these systems, because of the filling requirements of Euclidean space. The conflict between those two equirements must be relaxed by defects and it is the organization of defects which builds the crystal structures. The common features of these structures can be understood, if it is recognised that in each case ideal structures without defects can be built in the same curved space, the hypersphere S3, the packing requirements of which are compatible with the different local orderings of these various systems.

Introduction.

A structure results from a competition between local interactions and the topological or geometrical rules imposed by space filling requirements. When there is no disagreement between those two terms the structure can be readily understood, within classical crystallography, but this is not always the case, and the structure is then the result of a compromise more difficult to understand. For example, simple metallic atoms with short range isotropic interactions can build complex structures with large cell parameters and amphiphilic molecules, with a local liquid-like disorder, can build structures with long range crystalline order. We want to emphasize in this article that these two examples, as well as others, different in their chemical and physical natures, can indeed be understood within the same common frame. They are all systems in which the conflicts between local and topological constraints, frustration, cannot be relaxed totally by any configuration in Euclidean space. It is however shown that such configurations can be found in appropriate non-Euclidean spaces and that their knowledge is the key to the understanding of the structures observed. A most noticeable kinship exists between structures built by very different systems. Two simple 2D examples are helpful to get some feeling about the origin of the competition between local

and non-local rules and the way to relax it. First, consider a packing of discs on a plane with isotropic interactions organizing them in the most dense way possible, the discs being at the vertices of equilateral triangles. Clearly there is no conflict between the two rules, as a flat plane can be tiled regularly and compactly with the equilateral triangles. Let us now assume that the local interaction energy is a minimum when the discs are on the vertices of pentagons. If we now try to organize them on the plane, we discover that no regular long-range arrangement is possible. This is because a flat plane cannot be tiled with pentagons. In this second example there is obviously no compatibility between local and non-local rules, and the system is frustrated. If we insist on building a regular organization of discs at the vertices of pentagons, we are forced to change the non-local rule, abandoning the space of the plane for that of the sphere, since a sphere can be tiled with pentagons as shown in figure 1. In doing so, the frustration has been relaxed by changing the topology of the supporting 2D space. It could be argued that this is not very realistic, but the recently observed C_{60} molecule is an example of a 2D sphere tiled, in this case, with pentagons and hexagons. This ideal pentagonal structure in a curved space could be used subsequently for determining possible configurations in the flat plane, by mapping the curved space onto the flat space and introducing topological defects which perturb the structure locally and break the local rule. This is a necessary compromise to flatten the curved 2D space.
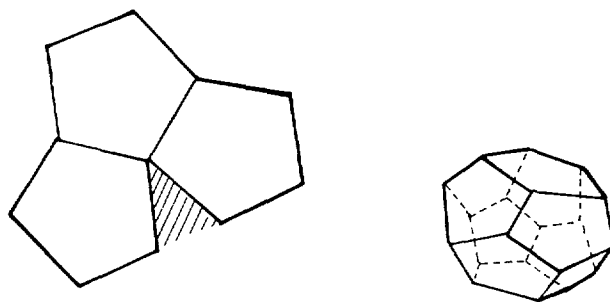

Fig. 1. — The flat plane cannot be tiled with regular pentagons whereas the sphere can.

This curved space approach was developed some years ago to explain amorphous metallic structures where the so-called « pseudo icosahedral » (« compact » or « polytetrahedral ») model was suggested by experimental results [1]. In this model metallic atoms are supposed to interact with a spherical potential, and therefore to pack 4 by 4 like spheres with their centers on the vertices of a tetrahedron but, on the long range, this order cannot propagate, since our Euclidean flat 3D space cannot be filled with regular tetrahedra. This is however possible in a curved 3D space and a complete description of the structure possible in the flat space is obtained once a network of adequate defects has been introduced to cancel the curvature of the curved space. This approach appeared helpful for other systems too, and we present here some structures in curved spaces which are now used to describe metallic alloys, tetra-coordinated semiconductors, as well as cholesteric blue phases and lyotropic liquid crystals.

Dense packing of spherical atoms.

If one tries to pack spheres in a dense manner by a discrete aggregation process, one easily finds that the regular tetrahedron, with one sphere on each vertex, is the best solution for 4 spheres, as shown in figure 2a. Then, going beyond 4 spheres and increasing the number of
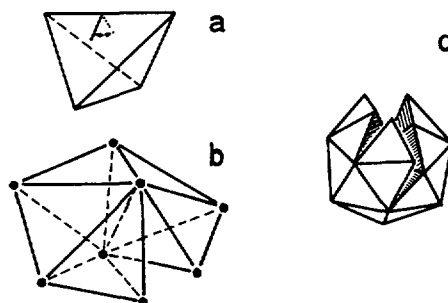
Fig. 2. — Regular tetrahedra do not tile the Euclidean 3D space, four atoms building a tetrahedron (a), five tetrahedra around one edge and the angular defect (b), an imperfect icosahedron of twenty tetrahedra (c).

tetrahedra, it soon appears that 5 tetrahedra share a common edge with a void between two triangular faces which cannot be filled, as shown in figure 2b, because the tetrahedron dihedral angle of 70° is not a submultiple of 360°. This misfit angle manifests itself again when one tries to propagate the local tetrahedral order around one vertex, and an imperfect icosahedron is obtained as shown in figure 2c.

TETRAHEDRAL PACKING AND THE {335} POLYTOPE IN S_3. — This misfit, which might be thought to be due to metric, is indeed more fundamental. Topology prevents the filling of the Euclidean space with regular tetrahedra. In order to overcome this imperfection, the first step consists in defining an ideal model in a space which can be filled perfectly with regular tetrahedra. This can be achieved in the spherical space S3, a curved space commonly known as the « hypersphere ». When embedded in 4D Euclidean space, the hypersphere has the equation $\sum x_i^2 = R^2$ with $i = 1$ to 4 and $R = (1 + \sqrt{5})/2$, if the tetrahedron edge length is the unity. The perfect tetrahedral packing on S3 is called the {335} polytope, a polytope being the equivalent of a polyhedron in higher dimensions [2, 3]. This polytope has a finite structure. As S3 is finite, it contains 600 tetrahedra and 120 vertices, there are 5 tetrahedra around a common edge with a perfect fit of the triangular faces, and 12 tetrahedra around a common vertex, in a perfect icosahedral configuration.

Some more ideas about the structure of this polytope can be conveyed using a simple 2D analogy. If we want to represent geometrical configurations drawn on the surface of a sphere on the Euclidean plane, as in cartography to represent the surface of the Earth on a map, we may use an orthogonal mapping, following which the set of circles parallel to the equator is mapped as a bundle of concentric circles onto a plane, tangent to one of the poles and, as long as the mapped region remains small around the pole, the configuration obtained on the plane is a rather faithful image of that on the sphere. In the case of the hypersphere orthogonally mapped onto a tangent hyperplane, a bundle of spheres concentric around the pole is obtained and, if a vertex of the polytope is chosen as a pole, the set of successive coordination shells is recovered after the mapping. But, as we are in 3D spaces, we can do this type of mapping not only in the vicinity of one vertex of the polytope but also in the vicinity of lines drawn by edges of the polytope. Among them is a great circle of S3, a geodesic of the space, it is drawn by 10 edges and is surrounded by tetrahedra enclosed in a torus bearing 50 vertices, as suggested in figure 3a. Thus, 60 vertices of the polytope, i.e. half of them, are organized on and immediately around this great circle, the other 60 are indeed organized in a similar manner on and around another great circle interlaced with the first, in a plane orthogonal to that of the first, as suggested in figure 3b. Those two circles are not only the axes of the two
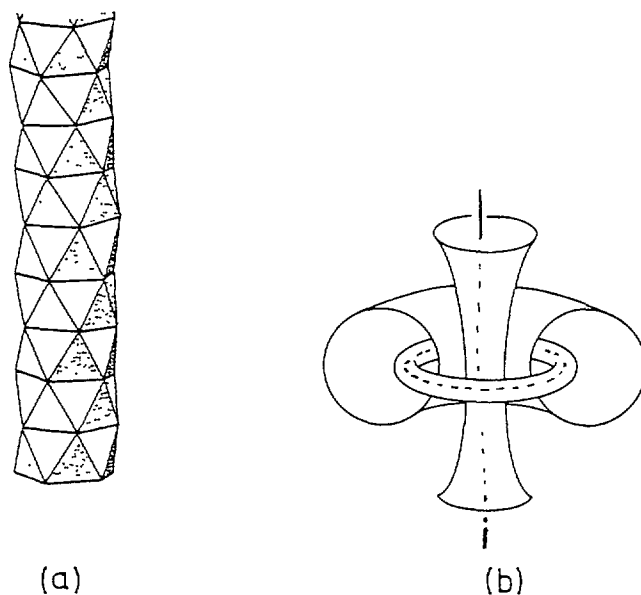
Fig. 3. — A column obtained by piling up pentagonal antiprisms, it can be decomposed into a tetrahedral packing (a), « flat » representation of the spherical torus at midway between the two interlaced organization of the circles and the two tori organized like in (a) ; in this representation one circle appears like a straight line, but in S3 both circles have the same radius (b).

tori bearing 50 vertices but also of a family of parallel tori contained in S3 to which the first two belong. One of the tori of this family is particular as it separates S3 in two identical subspaces spannig around the two interlaced great circles, it is called the « spherical torus » and will play an important role in many parts of this article. We may add that the spherical torus is a developable surface which is built in S3 by identifying 2 by 2 the opposite sides of a square flat sheet (an operation which is possible without distorsion in a curved space) and that the diagonals of this square, as well as all its lines parallel to them, become then great circles of S3. The parallel tori in the family, and particularly the two bearing the vertices of the polytope, can be built in a similar manner by identifying the opposite sides of rectangles of suitable side lengths.

CHANGE OF CURVATURE USING DISCLINATIONS. — Disclinations are Voltera's defects created by filling the lips of a cut in a structure with a wedge of material having a definite angle, or by removing a wedge from this structure and putting then the two lips together. A disclination is therefore a defect of rotation, while a dislocation is a defect of translation, and the resulting deformation corresponds to a change of curvature as the latter is characterized by an angle [4].

Adding a wedge of material to a structure in a spherical space decreases the curvature but structural defects appear along the edge and faces of the wedge. Nevertheless, if the two faces of the wedge are equivalent by a rotation belonging to the symmetry group of the structure, in our case that of the polytope, the defect is confined at the edge. A 2D example of a disclination is shown in figure 4. It is easy to observe how a disclination changes the curvature, and therefore the topology, in its immediate surrounding : a hexagon becomes a pentagon or a heptagon according to the sign of the curvature change. Disclinations can change rings formed by bonds between atoms, or change the coordinance of atoms, according to their relation with the positions of the atoms.
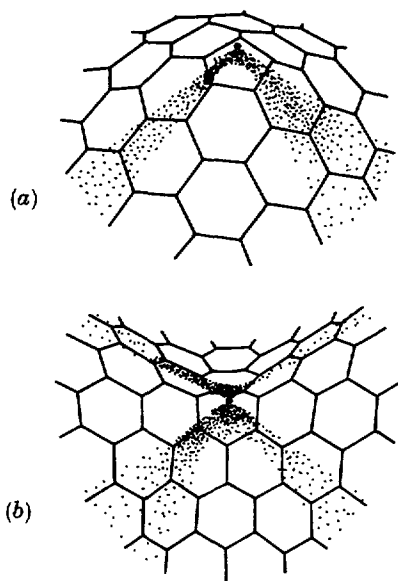
Fig. 4. — Disclinations in a hexagonal structure, a positive disclination (a), a negative disclination (b).

In a {335} polytope the local effect of a disclination running along some edges is to change the coordination number ($z = 12$) of points lying on the disclination line, as shown in figure 5 : the effect of a disclination on a structure being purely local, all other coordination polyhedra remain icosahedra [5]. The spherical torus allows a simple description of the effect of a disclination in the {335} polytope considering that, if the disclination runs along one axis of the torus, it changes the 5-fold symmetry of this axis into a 6-fold symmetry, for instance the torus represented in figure 3 as a piling up of pentagonal antiprisms becomes a torus built of hexagonal antiprism. A new polytope is obtained which contains 10 vertices on the disclination line, 6×10 vertices on the toric surface formed with hexagonal antiprisms, 12 vertices on the second axis of the torus and 5×12 vertices on the toric surface formed with
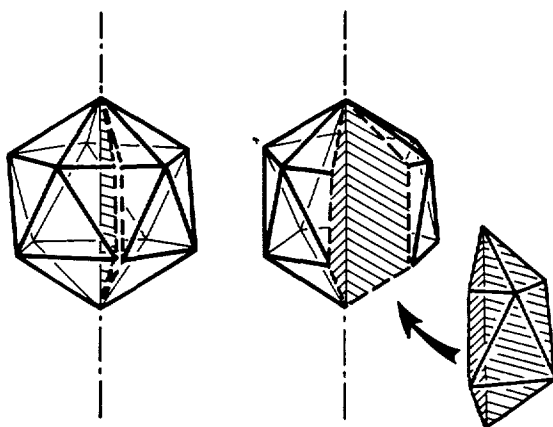

Fig. 5. — Procedure to insert a disclination (a), effect of a disclination on an icosahedral order building a $Z = 14$ coordination polyhedron (b).

pentagonal antiprisms around this axis. If, now, a second disclination is introduced along the second axis of the torus, the new polytope contains 24 vertices with coordinance 14 and 144 vertices with coordinance 12. The radius of curvature of S3 has increased from 1.618 to 1.93, in edge length unit. It is not yet infinite and more disclinations are to be added to decrease the curvature totally. The precise procedure is not well defined at the moment, we have described how to introduce one or two disclination lines in the {335} polytope but it is difficult, due to the non-commutativity of the symmetry operations associated with the disclinations, to insert disclinations one by one in order to flatten the structure. However, if a disclination network is generated with a symmetry group contained in that of the polytope, the difficulty may be by-passed [6].

STRUCTURES OF METALS AND METALLIC ALLOYS. — The {335} polytope, which provided a very fruitful approach of the icosahedral local order of pure amorphous metals, is also used to understand some particular structures of metals and alloys. In these cases tetrahedral interstices between atoms remain a reasonable hypothesis, even if the tetrahedra are no longer regular. We shall also shown that it is possible to put the largest atoms of an alloy on disclination lines to take the atomic size effects into account.

Metal structures are currently known te be b.c.c. or f.c.c. structures, with 2 or 4 atoms per unit cell, but there exist several cases with a larger number of atoms per unit cell which seemed at first very intricate. Most of these structures can be described by periodic networks of disclinations in a medium having the local order of the {335} polytope with one atom at each vertex. We give here two examples : the β phase of tungsten, with the so-called A15 structure, and a Laves phase.

The elementary cell of the A15 structure is a cube, an icosahedron with three orthogonal 2-fold axes superposed to the three 4-fold axes of the cube is inscribed in this cell so that there are 12 atoms on the face of the cube, a 13th at the center and 8 at the corners. There are therefore 8 atoms per cell, two with an icosahedral coordination (or W^b) and 6 with a coordination polyhedron having 14 vertices (or W^a). This polyhedron is identical to the coordination polyhedron of atoms lying on a disclination line as that shown in figure 5. In an infinite structure, a disclination line must have no end, and considering the situation of the W^a atoms we observe that the straight lines running through them and lying in the faces of the cubic cell can be defined as disclination lines, as shown in figure 6.

In a topological sense we may say that the structure of the β phase of tungsten in a {335} polytope with atoms on vertices and in which the disclination lines needed to flatten the space have changed the coordination polyhedron of three atoms out of four. This structure can be given the schematic formula $W^{a_3} W^b$ and, indeed, is also presented by several alloys with the same stœchiometry as for instance Nb_3Ge.
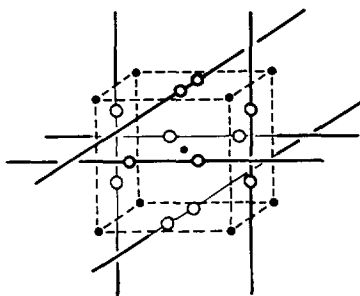

Fig. 6. — Disclination lines in the unit cell of the β-tungsten structure.

Laves phases, as for instance Cu_2Mg [7] are described by a cubic cell containing 8 atoms of one type, with a large Goldsmith radius, arranged like carbon atoms in a diamond structure and 16 atoms of a second type, with a smaller radius, filling the free space of the diamond structure. The coordination polyhedron for the second atoms is a slightly distorted icosahedron with 12 vertices, that of the first atoms has 16 vertices and can be obtained from an icosahedron by a disclination procedure in which 4 half disclinations are going to the center of the polyhedron or, equivalently, 2 disclinations intersect at the center, leading to 6 angles of 109°28'. The structure of the Laves phases can therefore be understood as originating from a {335} polytope which was flattened by a network of disclination lines organized in exactly the same way that the bonds of a diamond structure as shown in figure 7.
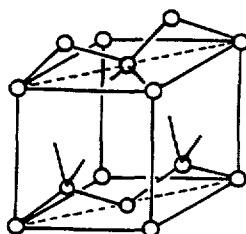

Fig. 7. — Disclination lines in the unit cell of the Laves phase structure.

These two examples of structures show how a local tetrahedral arrangement leads to structures with periodicities larger than the interaction lengths in order to account for topological constraints. It is always surprising to observe complex structures in simple metals and alloys between simple metals with isotropic atomic interactions but, because of the existence of a local interaction in a frustrated situation, these structures are structures of defects. This point of view extends the one developed for amorphous structures : a perfect structure in a curved space leads to a disordered structure or a crystalline structure with a large parameter in a flat space. Approximants of quasi-crystalline structures are related to this kind of alloys, for instance the AlMgZn structure was described as a structure of disclinations [8] and there are strong indications that it will be possible to describe quasi-crystals by this method also.

Tetracoordinated structures.

In covalent structures like a-Si or a-Ge, the short range order is perfectly defined by tetrahedral connectivity : one atom at the center of a tetrahedron is linked to its four neighbours by bonds directed towards the vertices of the tetrahedron. As this local order may lead to several different structures in flat or curved spaces it is necessary to add some details about the order at a scale slightly larger than the first neighbour distances [9]. The important topological ingredient for improving the description of the local order is the local ring configuration. A ring configuration is characterized by (i) the number of edges in the ring and its parity, (ii) the twist of the ring and (iii) the existence of cages with faces defined by rings or the non-existence of such cages. In dense and tetracoordinated structures the similarity of the local symmetry (tetrahedral interstices and bonds) leads to a relation between the two types of structures and this explains why we can obtain models for covalent structures starting from the {335} polytope and others derived from it.

THE {533} POLYTOPE IN S3. — If we put a vertex at the center of each to the 600 tetrahedral cells of the {335} polytope, and forget about the 120 original vertices, we obtain the dual polytope called {533} which contains 600 vertices and 120 cells which are regular pentagonal dodecahedra. Each vertex has a coordinance of 4, belongs to 4 dodecahedra and to 6 pentagons. The local configuration corresponds to the famous « vitron » of Tilton [10] and « amorphon » of Grigorovici [11]. The first two shells of vertices of the {533} are represented in figure 8. This structure is characterized by two important features : it contains 5-membered flat rings only and these rings enclose well defined dodecahedral cages. It is probably not a good model for a-Si or a-Ge but it can be used in order to understand the effect of 5-membered rings on, for instance, the electronic band structure [12].
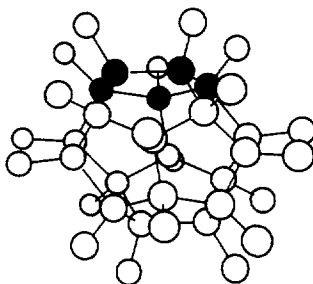

Fig. 8. — Part of the {533} structure, the closed circle shows a 5-fold ring.

THE « 240 » POLYTOPE IN S3. — There is another curved space solution to the tetracoordinated problem, a polytope which, in contrast with the {533}, does not possess all the {335} symmetry operations but only a subgroup. Its building rule is similar to that which generates the diamond network from the f.c.c. lattice. The diamond structure can be analyzed as being formed of two f.c.c. replicas displaced from each other in the {111} direction and the polytope « 240 » is similarly built from two {335} replicas but which are related by a screw symmetry operation in S3. Another way to obtain it is to place new vertices at the center of one out of five cells of the {335}, so that each vertex of one replica is surrounded by four vertices of the other. Consequently the polytope « 240 », with its 240 tetracoordinated vertices, is a « bicolor » structure with even-membered rings only. The smallest rings are hexagons in a twist « boat » configuration, as shown in figure 9, which preserves the perfect
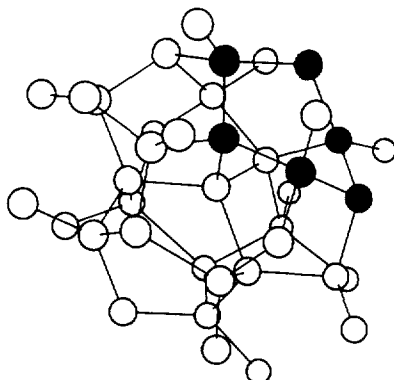

Fig. 9. — part of the « 240 » polytope, the closed circle shows a 6-fold twisted ring.

tetrahedral value for the bond angles but is associated with dihedral angle values intermediate between the staggered and eclipsed ones. The local order of this polytope is very close to the Connel-Temkin model.

Other polytopes with local order intermediate, between those of the {533} and « 240 », have also been proposed [13].

CLATHRATE STRUCTURES. — Ice associated with other molecules, such as rare gas, is the best known example for clathrate. In this case the tetracoordination holds to the electronic structure of the oxygen atom of one water molecule leading to the formation of two covalent bonds with its protons and two hydrogen bonds with those of two other water molecules. There are two types of structures which describe most of the clathrate hydrates [14] and which appear to be dual of the A15 structure (type I clathrate) and of the Laves phase structure (type II clathrate). In these structures the water molecules build cages, with oxygen atoms at the vertices and covalent and hydrogen bonds along the edges, trapping the associated molecules. The cages are defined by the edges of dodecahedra and disclinated dodecahedra, as shown in figure 10. These structures can be analyzed as {533} polytopes, the dual of the {335}, which have been flattened by disclinations, the disclination networks being similar to that of the β-tungsten structure in the case of type I clathrates or to that of the Laves phase structure in the case of type II clathrates.
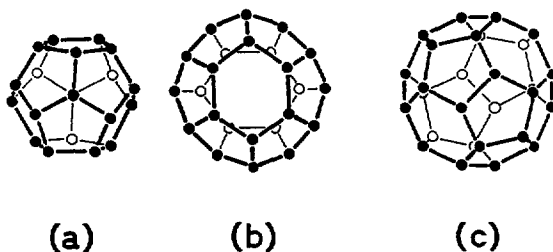

(a)   (b)   (c)

Fig. 10. — Cages in clathrates, a dodecahedron (a), a dodecahedron transformed into a tetrakaidecahedron by one disclination (b), a dodecahedron transformed into a hexakaidecahedron by four half disclinations (c).

There is another example of very interesting clathrate which complement the many types of structures formed by Si : no closed cages are observed in the crystalline form, they most likely do not exist either in the amorphous material but the compound $Si_{1-x}Na_x$ exhibits clathrate structures with cages built by the Si atoms and trapping the Na atoms when $0.02 < x < 0.2$, type I for large x and type II for small x [15]. These structures are good examples of structures built from amorphon with periodic disclination networks.

As well as beyond the A15 and Laves phase structures there exist other structures which can be described following the same approach, for instance β-uranium or Frank and Kasper alloys. There are also other clathrate structures with different connectivities of their disclination lines, for instance three in bromide hydrate instead of zero in type I or four in type II.

Cholesteric liquid crystals with double twist

These are assemblies of elongated organic molecules, without any long range translational order, but with a long range orientational order corresponding to a rotation of the mean molecular axis for any displacement orthogonal to it. As shown in figure 11, such an
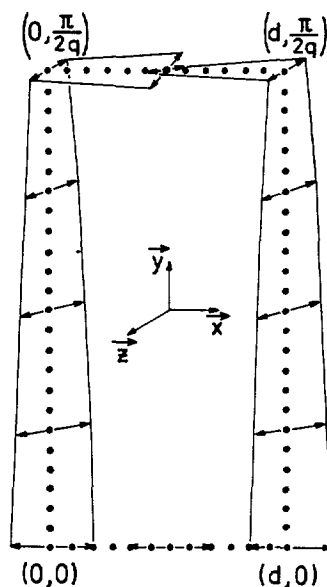
Fig. 11. — Frustration in « blue » phases. The director is supposed to rotate when it is displaced in a plane orthogonal to its direction. The director is along x at the origin, if it moves along two different paths towards a same point it will experiments two different orientations when arriving at that point.

orientational order cannot propagate without frustration in Euclidean space but, nevertheless, crystalline organizations called « blue phases » are observed. To describe them we make use of a particular set of lines in S3.

CLIFFORD'S PARALLELS IN S3. — They can be described from the toric decomposition of S3 discussed earlier, i.e. the family of parallel tori, all sharing the same orthogonal axes, which are obtained identifying the opposite sides of adequate rectangles, or a square in the case of the spherical torus which separates S3 in two identical subspaces. All these rectangles and square have the same diagonal length, which is that of a great circle of S3, and the anisotropy of the rectangles on either sides of the square of the spherical torus increases with their distance from it and, at the extreme, they become infinitely thin and confounded with the two orthogonal axes, as shown in figure 12. If we now draw, on each rectangle and square, lines parallel to its diagonal, these lines give in S3, after reconstruction of the tori by identification, a set of interlaced great circles, the so-called Clifford's parallels, such that any local orthogonal displacement from one to its neighbours is accompanied by a twist of the line, as suggested in figure 13. These lines clearly provide a solution free of any frustration for the double twist problem in cholesteric liquid crystals [16].
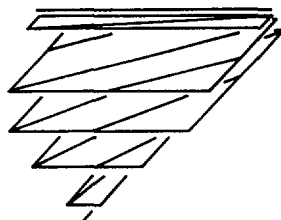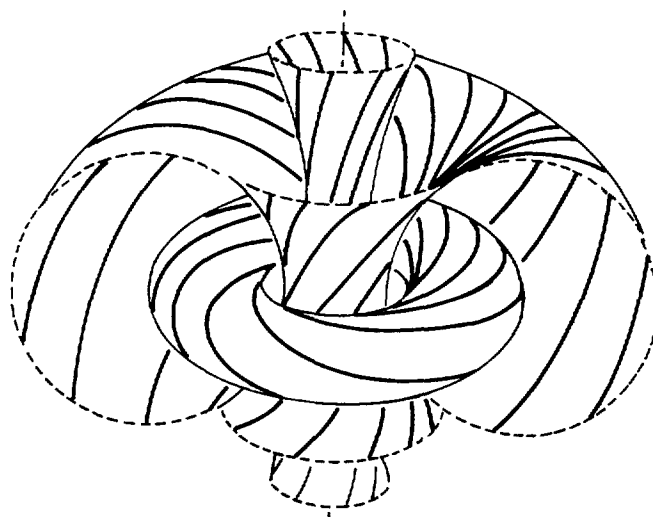

Fig. 12. — Rectangle representations of the tori in S3.

Fig. 13. — Stereographic mapping of the spherical space with Clifford's parallels.

PERIODIC STRUCTURES OF DISCLINATIONS IN « BLUE PHASES ». — As in other cases the curved space is then flattened by the introduction of disclination nertworks forming cubic structures similar to the A15 or Laves phase structures [17].

Cubic structures of liquid/liquid interfaces.

Periodic organizations of two fluid media separated by interfaces are very common in liquid crystals where they most often occur as stackings along one dimension of fluid layers of molecules, the so-called smectic phases. In the case of the lyotropic liquid crystals, built by amphiphilic molecules such as soaps, detergents and lipids, they are called lamellar phases and can be described as stackings of alternating layers of water and amphiphiles with flat interfaces defined by the polar heads of the amphiphiles, as shown in figure 14a. Besides these phases with periodicity along one dimension, the phase diagrams of these systems may present other ordered phases with periodicities along two or three dimensions, curved interfaces and complex topologies [18]. Here, we shall limit ourselves to the cases of structures with cubic symmetry, which are known to present two topologies, bicontinuous and micellar.

A few phase diagrams of amphiphilic molecules in the presence of water exhibit cubic structures in two distinct concentration domains [19, 20]. Some of them are observed in the vicinity of the lamellar phase. They are now well characterized, their space groups being Ia3d or Pn3m in most cases, Im3m in some others and they can be described as being built by two interwoven labyrinths of one medium separated by a film without self-intersection of the other, as shown in figure 14b, hence the characterization of their topology as « bicontinuous ». The other cubic phases are observed in the vicinity of the micellar phase, their space groups are Pm3n, Fd3m or P4332 [21], their structures are not as well characterized as those of the bicontinuous cubic structures at the moment. Because of their location in the vicinity of micellar phases, far from the lamellar phase, they were not expected to have a bicontinuous topology. However, arguments from NMR were in favor of structures built with finite micelles of one medium separated by a self-intersecting film of the other [20], as shown in figure 14c, hence the proposition of a cellular or « micellar » topology.
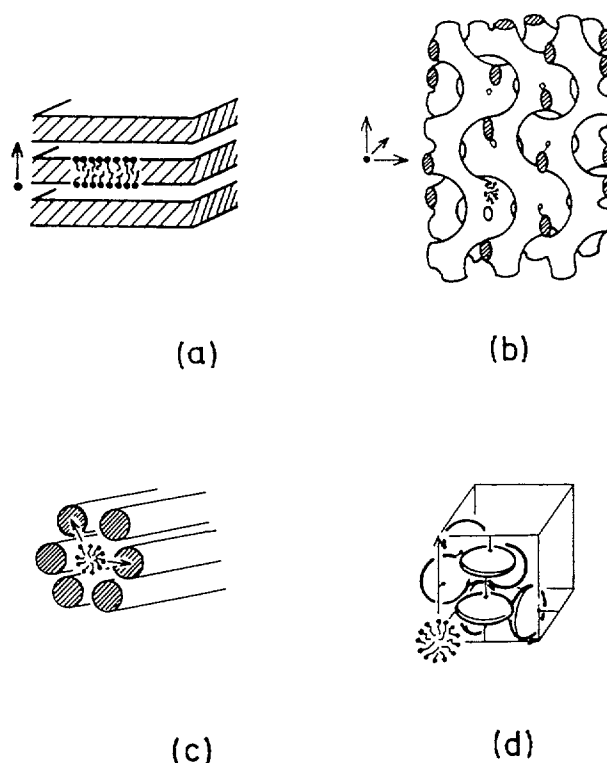
Fig. 14. — Structures built by amphiphiles, lamellar (a), « bicontinuous » cubic (b), hexagonal (c) « micellar » cubic (d).

THE FRUSTRATION AND ITS RELAXATIONS. — There are several forces stabilizing such systems of interfaces, which are not all well known at the moment. Fortunately we do not have to consider them in full detail for the rest of our presentation. We just need to know that there are forces normal to the interfaces, which control the distances between interfaces, and forces parallel to the interfaces, which control their curvature as in a bi-metallic switch, because the lateral area occupied by the chains do not vary necessarily in the same way as that of the polar heads. Owing to the fact that the bilayer of amphiphiles admits a plane of symmetry it is clear that a non-zero curvature of the two interfaces is not compatible with constant distances between them if the lamellar symmetry is kept, as shown in figure 15. The
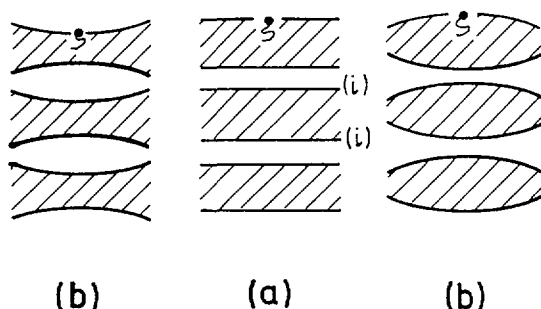

Fig. 15. — Frustration in systems of films, flat interfaces are compatible with constant distances between interfaces (a), curved interfaces are no longer compatible with constant distances (b).

normal and parallel forces are therefore in conflict : this is a typical state of frustration which can find no solution in our Euclidean space.

This frustration may indeed be relaxed if the system is transferred into the curved space S3, the film of two interfaces being supported by surfaces of this space respecting its symmetry, i.e. separating S3 in two identical subspaces. There are indeed two such surfaces in S3, the spherical torus already described and the great sphere [22].

GENERATION OF THE BICONTINUOUS TOPOLOGY [23]. — From the properties of S3 and its family of parallel tori it appears that the set of the spherical torus surrounded by two parallel tori at equal distances on either sides of it can be considered as a representation without frustration of the periodic system of fluid films which is frustrated in Euclidean space. The periodicity in this space, which is the repetition of the films when moving along the geodesics of the space normal to the films, is reproduced in the curved space by the displacements along great circles of S3 normal to the tori. Moreover, as already said above, the two subspaces separated by the spherical torus are identical, as are two spaces separated by the film in the cell of the structure and, finally, the frustration is obviously relaxed as the two tori parallel to the spherical torus have a smaller area.

The possible geometrical configurations in Euclidean space are to be found by mapping S3 onto it, as usual now. We limit ourselves to the process which maintains the bicontinuous topology of the spherical torus, as suggested in figure 16 where one $-\pi$ disclination was introduced along a C2 symmetry axis of the spherical torus. In the course of this process the positive curvature of S3 is decreased to zero and the spherical torus, which is a surface with zero Gaussian curvature in S3, becomes a surface with negative Gaussian curvature in Euclidean space, as are the surfaces separating the two labyrinths of the cubic structures. The possible symmetries of these surfaces are also imposed by those of the spherical torus and the disclinations.
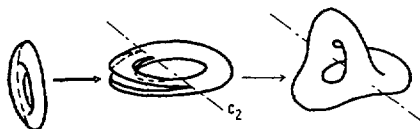

Fig. 16. — Deformation of the spherical torus with genus 1 into a torus with genus 2 by a $-\pi$ disclination along a 2-fold axis.

GENERATION OF THE MICELLAR TOPOLOGY [24]. — In this case we use, as a supporting surface for the film of amphiphiles in S3, the second surface separating S3 in two identical subspaces. This surface is a great sphere S2, which can be considered as the exact equivalent in 3D of the equator drawn on a 2D sphere and separating it in two hemispheres. As, on the 2D sphere, there is a family of smaller circles parallel to the equator with their centers at the poles, there is, in the 3D sphere S3, a family of smaller spheres parallel to S2 with their centers at the poles of S3. Thus, the large sphere S2 with two parallel spheres at equal distances on each side can be considered as another representation without frustration of the the periodic system of fluid films which is frustrated in Euclidean space. The periodicity in this space, which is the repetition of the films when moving along the geodesics of the space normal to the films, is reproduced in the curved space by the displacements along large circles of S3 normal to S2, moreover, as already said above, the two subspaces separated by the large sphere are identical, as are the two spaces separated by the film in the cell of the structure

and, finally, frustration is obviously relaxed as the two spheres parallel to the large sphere have a smaller area.

The mapping onto the Euclidean space of this relaxed structure in its curved space is done by introducing $-\pi$ disclinations around its C2 symmetry axes which are large circles of S2. The effect of one disclination is shown in figure 17, it brings in a third finite subspace. The introduction of the network of disclinations needed to suppress the curvature should extend the number of identical subspaces to infinity, thus creating a structure of finite cells whase topological stability implies that the walls limiting them meet three by three along common edges which meet four by four at every vertex. Unfortunately there is no assembly of identical cells obeying these laws in Euclidean space [25], we can find them in curved spaces only. If we search for the assembly possible in the space with lowest curvature, which will therefore be considered as a step in the flattening process, we find that of regular dodecahedra, which we have already met as the {533} polytope in the case of clathrates particularly. The last step for flattening is therefore already known and leads to structures with the same symmetries as those of clathrates, i.e. those of the A15 and Laves phase structures. We recall that these structures are non regular assemblies of polyhedra but, in this case, the faces of the polyhedra support the film which limits the cells enclosing the micelles of amphiphiles. The two structures are shown in figure 18, from [26]. One, related to A15 and type I clathrates, has space group Pm3n and its unit cell contains two dodecahedra and six tetrakaidecahedra, the second, related to the Laves phase and type II clathrates, has space group Fd3m and its unit cell contains sixteen dodecahedra and eight hexakaidecahedra.
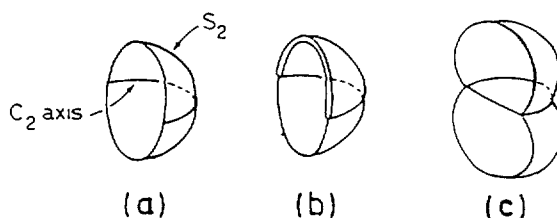

Fig. 17. — Effect of a $-\pi$ disclination along a 2-fold axis of a great sphere S2 of S3. The S2 sphere (here represented by a half sphere) separates S3 in two cells (a), the inside and the outside on this schematic representation. The disclinated surface separates S3 in three cells (c).
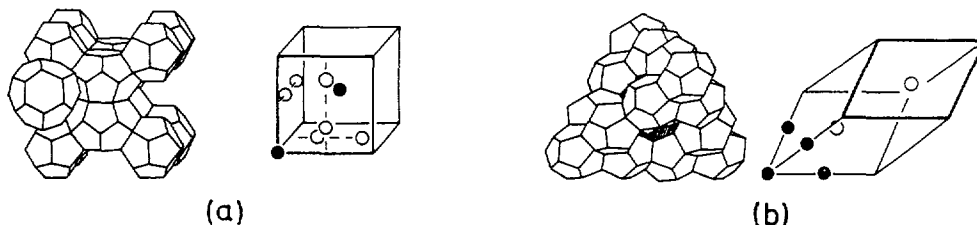

Fig. 18. — Two « micellar » cubic structures, Pm3m (a), Fd3m (b).

Conclusion.

We have considered several systems which, in spite of very different chemical and physical natures, present very strong structural similarities. They all have cubic cells, with related symmetries and parameters larger than the typical interaction distances. The reasons for this

are not easy to grasp if one considers that the basic structural elements, atoms in metals and alloys, molecules in clathrates, directors in cholesteric liquid crystals and liquid films in liquid crystals of amphiphiles, have no common features. However, precise analysis of local interactions and space filling requirements showed that all these systems shave one property. They cannot build perfect organizations of their structural elements in Euclidean space since the propagation of their local order would not be compatible with the topology. Thus, the extension of the local order is necessarily limited up to a distance at which the resulting stress becomes too large and defects appear within the materials. We have presented a systematic approach to the origins and the natures of these defects and we showed that the structures observed must indeed be seen as structures of defects, more exactly organizations of lines of disclination with particular topological properties. The relationships between these very different systems, therefore, are of this nature.

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