GEOMETRIES AND INTERFACES
A. Mackay

To cite this version:
A. Mackay. GEOMETRIES AND INTERFACES. Journal de Physique Colloques, 1990, 51 (C7), pp.C7-399-C7-405. <10.1051/jphyscol:1990739>. <jpa-00231138>

HAL Id: jpa-00231138
https://hal.archives-ouvertes.fr/jpa-00231138
Submitted on 1 Jan 1990

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L’archive ouverte pluridisciplinaire HAL, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d’enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.
GEOMETRIES AND INTERFACES

A. MACKAY

Department of Crystallography, Birkbeck College, University of London, Malet Street, GB-London WC1E 7HX, Great-Britain

Abstract

This conference has shown that the topic of Geometry and Interfaces has congealed as a distinct subject area, perhaps to be called flexi-crystallography. As well as considering liquid crystals, it includes a large class of materials, natural and synthetic, which are not regular three-dimensional crystals, but which nevertheless have considerable order. Among these can be distinguished curved two-dimensional manifolds, some of which can be patched into crystals. New geometries, including those of $S^3$, $H^2$, $H^3$, $T^2$, becomes relevant, being made visible by computer graphics. Some representations, particularly periodic minimal, equipotential and nodal surfaces also illuminate the structures and properties of regular crystals. These surfaces, on various scales, can be discerned in materials by using microscopy and less direct techniques.

Crystallography is not enough. The great success of the paradigm of X-ray crystal structure analysis in imaging crystal structures[2] has led to a knowledge of the shapes of 100,000 molecules and of some 10,000 ionic and metallic crystals. The price paid for this information includes the assumption that all the unit cells in the crystal are identical. This price is required by the methods used to recover the lost phases of the sine waves which go to make up a picture of a crystal structure. However, high resolution electron microscopy and scanning tunnelling microscopy are now developing and are increasingly capable of imaging general, non-repeating objects to atomic resolution. Most biological structures are not crystalline. In crystals one rule of composition carries the structure from the atomic level to the scale of centimetre crystals, but in biological structures the characteristic feature is hierarchy - after only a few repetitions a new building rule for the larger units appears.

Moreover, living organisms exhibit the building principle which François Jacob called bricolage. Complete sub-assemblies, evolved for some other organism, associate and may achieve a symbiosis, forming some larger organism. In particular, the eucaryotic cell seems to have been a symbiosis of smaller, originally independent, organelles. Even inorganic systems may become incorporated, if they are advantageous, and turned to quite surprising 'purposes'. An example is the use of magnetite crystals, presumably once a degradation product, in magnetotactic bacteria, where they direct the bacteria towards or away from a congenial anaerobic environment and are accordingly favorable or unfavorable to survival and reproduction.
Liquid crystal systems can be seen as the first steps away from crystalline regularity. So also are the irrational alpha-helix of Linus Pauling, the double helix of DNA, the icosahedral virus particles, first seen by Rosalind Franklin in poliomyelitis virus and the icosahedral quasi-crystals found in Al/Mn and other alloys.

All these structures can be seen as conflicts between local order and the long-range order which is necessary for crystals. The most general geometrical relationship between two identical particles complex enough to have non-central forces, is a helix, a combination of a translation and a rotation. These are usually irrationally related - the translation is associated with an irrational fraction of a turn.

Similarly, when three or more complex particles associate, they do not generally define a plane but part of a curved surface, which is usually incompatible with the regular translations needed to form a crystal. When the Gaussian curvature of the surface is positive, finite closed shells, as in the icosahedral viruses, result. However, when the Gaussian curvature is negative, each patch is locally saddle-shaped, and the structure can continue indefinitely.

It has been the realisation that patches of negative curvature can be joined together to give structures with crystalline repetition in three dimensions which has enlivened the field of the study of membranes and lyotropic liquid crystals and has led to the present conference where periodic minimal surfaces — PMS — take the most important role.

The book *Structure in Nature is a Strategy for Design* by Peter Pearce has been influential in bringing PMS and other structures to the notice of scientists and designers.

1 Geometric invariants

In pursuing the aim of Felix Klein in his *Erlanger Programm* to develop geometry in terms of invariants which do not depend on arbitrary axes, we can recognise invariant shapes which are used in, for example, the description of coordination polyhedra[13]. Everyone needs to know the five Platonic regular solids and the thirteen Archimedean semi-regular solids. Crystallographers recognise the regular *forms* of crystal faces. We now need to add the principal periodic minimal surfaces to this list.

2 Surfaces

There has been a tendency to see the structure of materials, at the level of the arrangement of atoms in space, in terms of bonds between atoms and to build physical models with balls joined by spokes. This is certainly good for most molecules but it is less satisfactory for ionic and metallic structures, where bonds are not clearly defined, nor in the interactions of macro-molecules, where hydrophobic and hydrophillic regions are important. Surfaces of various kinds are now seen to be important and computer graphics have provided possibilities of visualising them.
2.1 The division of space

In arrangements of atoms (or other units) space can be divided in various ways so that a domain is allocated to each atom. The Voronoi and radical plane dissections[6], the latter now sometimes called after Laguerre, have been widely used. They have the advantages of allocating all space to one or other domain, giving convex domains with plane faces, within which all points are nearer to one atom than to any other. In the Voronoi dissection all faces are the perpendicularly bisecting planes of lines joining pairs of atomic centres. In the Laguerre dissection, of which the Voronoi dissection is a specialisation, the atoms are given finite radii and the planes are the radical planes, the loci of points with equal tangent distance to two atomic spheres.

There are various ways of calculating such surfaces: (a) exact accountancy[5], solving for the centres of the spheres circumscribing all sets of four points, which become the vertices of the polyhedra. This method is tedious and exacting if there is high symmetry. (b) set theory methods exemplified by that of Brostow, Dussault and Fox[3]. (c) statistical methods which take pixels (or voxels) at random, or simply all pixels, and by brute force find which atomic centres are nearest to them[1]. These methods are very simple and adaptable to very general definitions of potential. They can be applied also to geography and economics.

There is an associated division into tetrahedra, the Delone tessellation, where the vertices are the atomic centres and the vertices of the Voronoi polyhedra.

3 Periodic minimal surfaces

There are two types of periodic minimal surfaces without self-intersection (a) where the two subspaces are congruent (Identical or mirror images). These are called balance surfaces by Fischer and Koch who have enumerated and described the complete set of such surfaces. (b) The two subspaces may be non-congruent, in which case the number of surfaces existing may be indefinitely large. It seems probable that fractal, quasi-periodic and statistical surfaces can exist, since “reasonable” topological models can be produced, but this will require more careful analysis.

Minimal surfaces, with zero mean curvature everywhere, make the splay energy zero and minimise the area of each element of area. If other energy functions are involved the surface may be somewhat different. Thus, periodic minimal surfaces are important in representing clear geometrical invariants but are not necessarily the exact shapes which may be appropriate in a particular physical case. Periodic minimal surfaces, periodic nodal surfaces and zero equipotentials may be very similar in certain cases. In physical cases such as a membrane bilayer or a layer of amphiphilic molecules between oil and water regions, the interface is relatively thick and for real cells the elastic properties of the cell membrane are complex, being further complicated by the presence of the cell cyto-skeleton. PMS with a standard nomenclature afford clear descriptions of the topologies of interfaces which can then be qualified.

Surfaces closely similar to PMS occur at a range of scales:
(a) at the atomic level the surfaces of zero equipotential which divide zones of positive potential from those of negative potential in ionic structures, the simplest of which is CsCl;
(b) at the molecular level in lyotropic liquid crystals. Here the geometrical problem is extended, as shown by the work of Brigitte Pansu and Elisabeth Dubois-Violette on the blue phases, towards the mapping of the line of the director in liquid crystals on to surfaces.
(c) at the macromolecular level in the interfaces between polymers. Here Edwin Thomas has shown, since the scale is suitable for electron microscopy, that the interfaces can be directly observed.
(d) at the cellular level in the topology of cells in the earliest stages of embryogenesis, for example in gastrulation.
(e) as engineering structures, ranging in size from electronic devices through heat exchangers to buildings.

Yves Bouligand and Françoise Gaill have demonstrated that in biological organisms there is an enormous range of remarkable structure and that this remains the richest field of exploration. The novelty of our imagination is often exceeded by the ingenuity of nature.

3.1 Construction of PMS

Periodic minimal surfaces can be constructed in a variety of ways, some of which are described in more detail elsewhere in this volume.

Surfaces may be described in the notation of Monge as \( z = f(x, y) \) or, more generally, as \( f(x, y, z) = 0 \). \( x, y, z \) may themselves be functions \( x = x(u, v), y = y(u, v), z = z(u, v) \) of parameters spanning the surface. The Monge form is seen to be a simple case of this parametrisation. Difficulties in using it may occur if, in the coordinate system chosen, the surface has anywhere an infinite gradient. Derivatives may be abbreviated as: \( \frac{\partial f}{\partial x} = f_x, \frac{\partial^2 f}{\partial x \partial y} = f_{xy}, \) etc.

The expressions for the mean and Gaussian curvatures, \( H \) and \( K \) are:

\[
H = \frac{(1 + f_y^2)f_{xx} - 2f_x f_y f_{xy} + (1 + f_x^2)f_{yy}}{2(1 + f_x^2 + f_y^2)^{3/2}}
\]

This is the Laplace-Young equation. When the gradients are small it reduces to the Laplace equation \( f_{xx} + f_{yy} = 0 \).

\[
K = \frac{(f_{xx} f_{yy} - f_{xy} f_{xy})}{(1 + f_x^2 + f_y^2)^2}
\]

The mean curvature \( H \) of an element of surface described as \( z = f(x, y) \), using the Monge notation, is given by this Laplace-Young equation. Thus the surface satisfied this partial differential equation everywhere.

(a) The Weierstrass projection operates in two stages: a point in the complex plane is projected stereographically on to a sphere, this point is then projected to three-dimensional coordinates to give the point in space where the surface normal has the same direction as the normal to the corresponding point on the sphere. The projection involves integration
of a complex polynomial which is constructed from a knowledge of the coordinates of the flat points on the surface.

(b) Finite element analysis can be used to improve an approximate surface to fit any required conditions on its curvature. More general conditions than $H=0$ which corresponds to zero splay energy can be incorporated, if the surfaces are postulated to have more complex elastic characteristics.

(c) In many cases distributions of positive and negative charges can be found which give periodic contours of zero electric potential which are close to periodic minimal surfaces. Von Schnering and Nesper have given a useful table[12].

(d) Actual experiments with soap films are by no means to be despised and there is scope for precise experiments to determine critical ratios and also to measure the elastic constants of films. In the (tetragonal) T-surface the symmetrical solution should obtain whatever the $c/a$ ratio. Preliminary physical experiments indicate that the soap film may have an energy which also includes a term in the Gaussian curvature since for $c/a=4$ the symmetrical solution bifurcates into two less symmetrical solutions.

3.2 Surfaces of constant $H$

The same methods used for constructing PMS, where $H=0$, can be used for constructing parallel surfaces where $H=\text{constant}$. These correspond to soap bubbles where there is a pressure difference proportional to $H$ across the film. The energy is proportional to $H^2$.

3.3 Periodic nodal surfaces

The development of periodic nodal surfaces by Von Schnering and Nesper and by Mackay, represents a step with potential implications for crystallography generally. It began with J. W. Cahn’s representation of spinodal decomposition [4] by the zero contour of sine waves with random direction, amplitude and phase but with the same wavelength. This gives a good picture of an emulsion with an average mean curvature of zero. It would be of interest to calculate the mean value of $H^2$ for this since it would be proportional to the splay energy. Fermi surfaces are conventionally generated as the zero contours of the sum of a number of low order Fourier terms, usually all of the same form \{hkl\}. It was recognised that this method gave a quick approximate picture of a variety of periodic minimal surfaces corresponding to the zero equipotentials of a variety of charge distributions [12]. The algebraic forms used are in fact those listed in K. Lonsdale’s structure factor tables [7]. The zero contour for the

$$C(\vec{r}) = \sum_{\{hkl\}} F_{\{hkl\}} \exp(2\pi i \vec{h}_{\{hkl\}} \cdot \vec{r})$$

is a kind of crystallographic invariant shape. Such functions are members of orthogonal sets. Being sums of cosine waves which are linked together by symmetry-related phases, as members of a common form \{hkl\}, if the structure amplitudes of that form are large, the nodal surface is of structural significance. The phases may be related to others by the direct methods of Karle and Hauptman.
4 A Databook on Surfaces

One of the results of this conference should be to produce a simple data booklet to make the results of the work described accessible to other, less closely concerned, scientists who are not in a position to assimilate the more technical books of the Orsay\cite{11} and Canberra\cite{10} groups.

Already the geometry of minimal surfaces has caught the imagination of several artists and in particular Patrice Jeener \cite{8} has produced a collection of etchings, valuable in promoting familiarity with the various geometrical objects.

5 The emergence of a subject area

The Science Citation Index provides measures of the connectivity of the network of scientific papers. Two contemporary papers are connected if they cite the same ancestor. This cross-citation criterion discerns groups of papers which cite each other heavily and also cite common ancestors. It may show that a cluster of papers is more strongly connected within itself than to other regions of science and thus that a new subject area has developed. It has been shown that the metaphor of \textit{areas, frontiers, neighborhoods, fields of science} is well based and that, by taking the two largest eigenvalues of a suitably normalised distance matrix, these clusters of papers can be mapped quite well onto a two-dimensional plane. Thus, science itself has been shown, notably by D.J.de S. Price and Eugene Garfield (of the Institute of Scientific Information), to have a structure. It is to be expected that the new grouping represented by the individuals concerned with the Aussois meeting and their papers will soon show up in the literature as a distinct new department of science.

This new department appears as the union of parts of \textit{mathematics} (aided by computer graphics), \textit{crystallography} generalised to curved manifolds and \textit{liquid crystals} (which occur both naturally and synthetically).
References


