Colouring 2D Polycrystals

A dense packing of the Voronoi polygons (VP) was created by the Centroidal Voronoi (CV) iteration. It includes VPs with 5, 6 or 7 sides. VPs are represented in a dual triangular representation. In this way, a polycrystal containing grains made of hexagons is formed. The grains are separated by lines of 5/7 pairs. To emphasize the orientation of the grains, we colour the edges of triangles according to a saturated colour circle (CC). The colouring depends on the edge direction modulo 60 degrees. Thanks to this, the colour of edges of an equilateral triangle is the same. Since the colours give the direction of the edges, the colours of the edges of the pentagon go in the opposite direction to the colours of the edges of the heptagon. Thus the CV iteration leads to uniform packing and to the famous hexatic phase transition.

Keywords: *Voronoi's polygon, duality, Colour Circle, 5/7 dislocation, film*

Introduction

Our results presented below are based on research presented at the MIT Conference in 1970, hereinafter referred to as [MIT Conference 1970]. We then produced two dimensional (2D) polycrystals by Centroidal Voronoi (CV) iteration. Polycrystals have been shown to consist of grains and a 5/7 (pentagon/ heptagon) dislocations. At the same conference, Cyrill Smith described changes of grains in a polycrystal, [Smith 1970].

The issue discussed below below pertains to the mathematical problems of packing, i.e. the optimal arrangement of objects in a container. In our case, it is about the possibly ordered arrangement of atoms in the crystal lattice. Optimization is carried out using a geometrical version of the successive approximation method, known as the Voronoi iterative method.

Voronoi Polygons and its Dual Triangulations

The Voronoi polygon (VP) consists of all points of the plane closer to a given center than to any other center, (Voronoi 1909). In practice, we divide the segments connecting the adjacent centers in half, run perpendiculars to these segments at the dividing points and connecting them we get VPs, see Fig.1. The dislocation pentagon-heptagon (5/7 pair) is the smallest pair of Euler's polyhedral law, [Cahn 1970].

The dual to the Voronoi polygons is the Delone triangulation, in which the vertices are connected by triangle edges to neighbouring vertices, see Fig.2, [Delaunay 1934].

In Plato's *Timaeus*, symmetrical polyhedra are described, among which the dodecahedron and the icosahedron are related by the duality relation. The dodecahedron is made of 12 equilateral pentagons. It has a dual triangulation with an icosahedron made of 20 equilateral triangles.

Figure 1. *(a) Some arrangement of scattered centers (e.g. atoms) in the plane. (b) Voronoi polygons (in red) correspond to the arrangement in (a): points inside a Voronoi polygon are closer to its center than to any other center. The 5/7 pair is visible in the middle of the figure (b)*

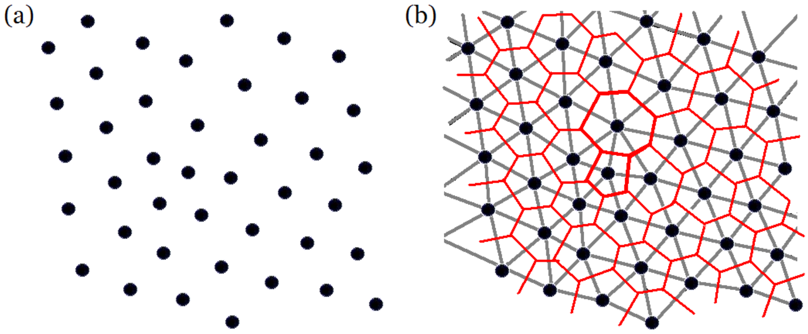
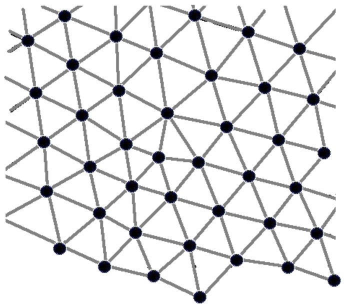


Figure 2. *Delone triangulation corresponding to the Voronoi polygon tessellation in Fig. 1b*



Method

Centroidal Voronoi Iterations

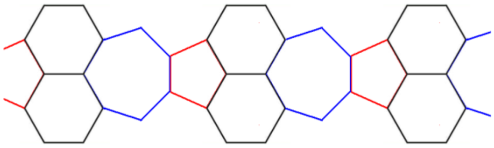
Centroidal Voronoi (CV) iteration method consists of three steps; 1: determining centroid of VP, 2: constructing new VP from centroidal centers, 3: goto 1. CV was first presented at the conference on Computer Films for Physics, Boulder Colorado 1978; also [Lissowski, Wojnar 2001].

These iterations lead to more regular close packing of 5, 6, and 7 (penta-, hexa- and septagons). Gradually the number of 5/7 dislocations is decreasing, and in consequence the grains of 6 (hexagons) are growing.

Grain Boundaries

The polycrystal consists of grains, and the grains are made of the equilateral triangles with similar side directions modulo 60º. The dislocation pairs 5/7 are aligned along grain boundaries (GB), Fig. 3, [Gleiter, Lissowski 1971]. Sometimes three boundaries meet at triple junctions.

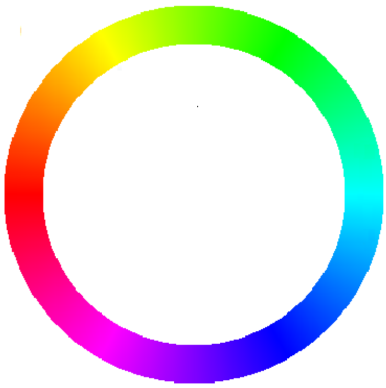
Figure 3. *In this example the grain boundary consists of successive pairs of 5/7s separated by a transverse pair of two 6s [Gleiter, Lissowski 1971]*



Colouring

We use the saturated Colour Circle (CC), see Fig.4.

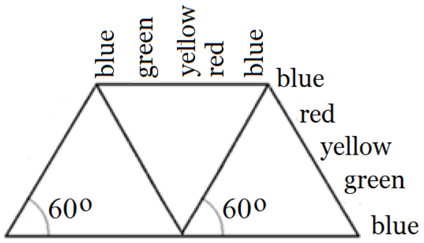
Figure 4. *Colour circle showing fully saturated colours*



A colour from this Circle is assigned to each edge of triangle, depending on the direction of the edge, measured modulo 60º. Thus, the colours repeat every 60º, cf. Fig.5.

Of course, one can assign any colour to the zero direction (for example, the direction of the abscissa), and then consistently assign colours to other directions in the order in the CC.

Figure 5. *Correspondence of directions and colours. The entire range of colours is within an angle of 60º, and the colours repeat modulo 60º. In this case the direction zero degrees is attributed to blue*



Description of 2D polycrystal

Figures 6 and 7 show examples of crystallization. The change in crystallization directions of adjacent grains is proportional to the 5/7 dislocation density at the boundary between these grains.

Figure 5. *An example of crystallization by the CV iterations. Black circles denote pentagons (5) and white circles denote heptagones (7). Chains of 5/7 dipoles mark grain boundaries. The boundaries are more pronounced the denser the dipoles appear. Note that dipoles on grain boundaries are always arranged in one direction, and the fives are always close to the sevens*

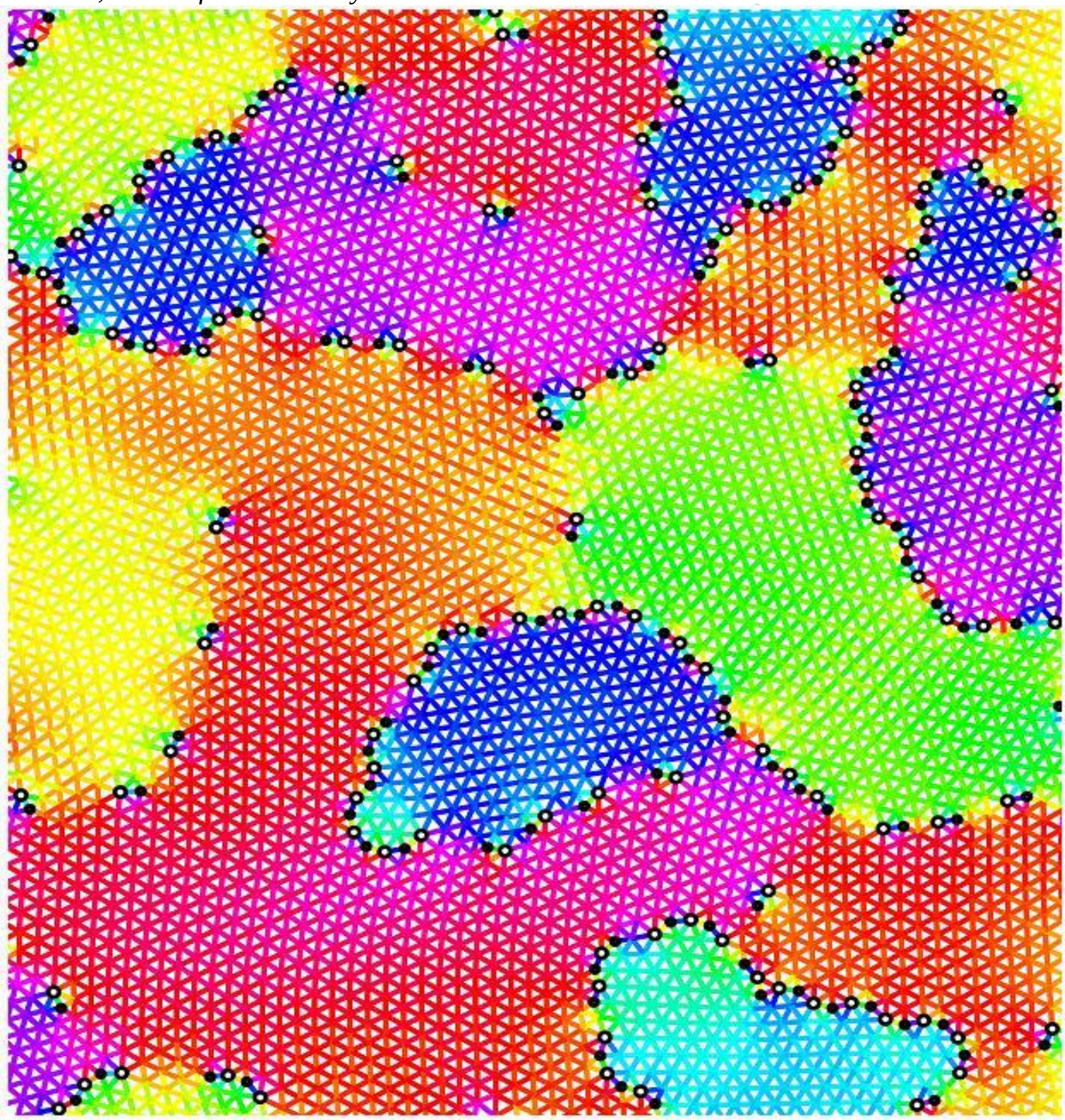
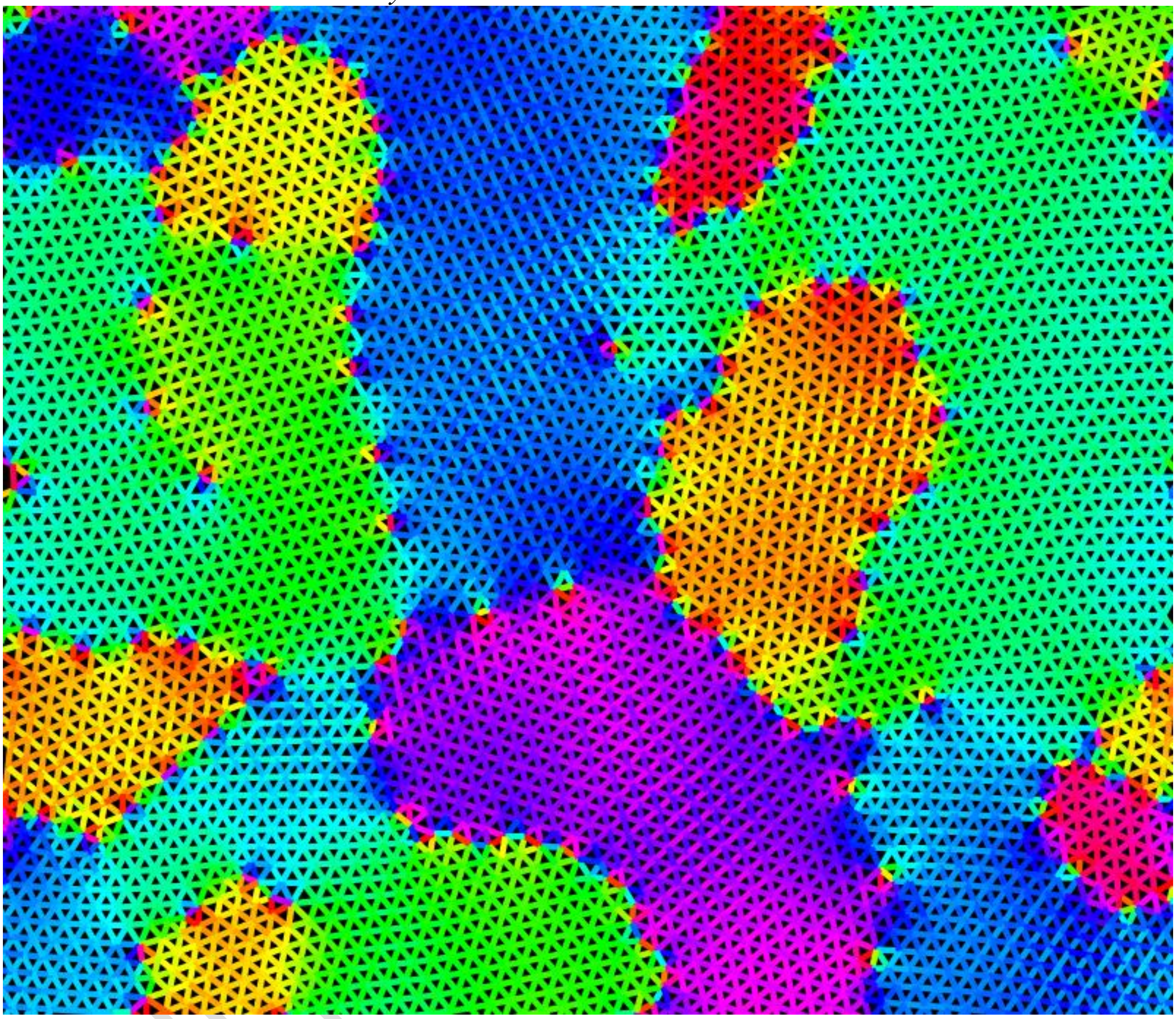


Figure 6. *Another example of crystallization by the CV iterations. Color vortices around dislocation 5/7 are clearly visible*



Instead of colouring only the edges of the triangles, one can colour each entire triangle with the average colour of its 3 edges. Examples of such colouring can be seen in Figs.7 and 8

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Figure 7. *Each triangle of the Delone triangulation is obtaining the average colour of its edges. Dipoles 5/7 stand out with a different colour, and define grain boundaries*

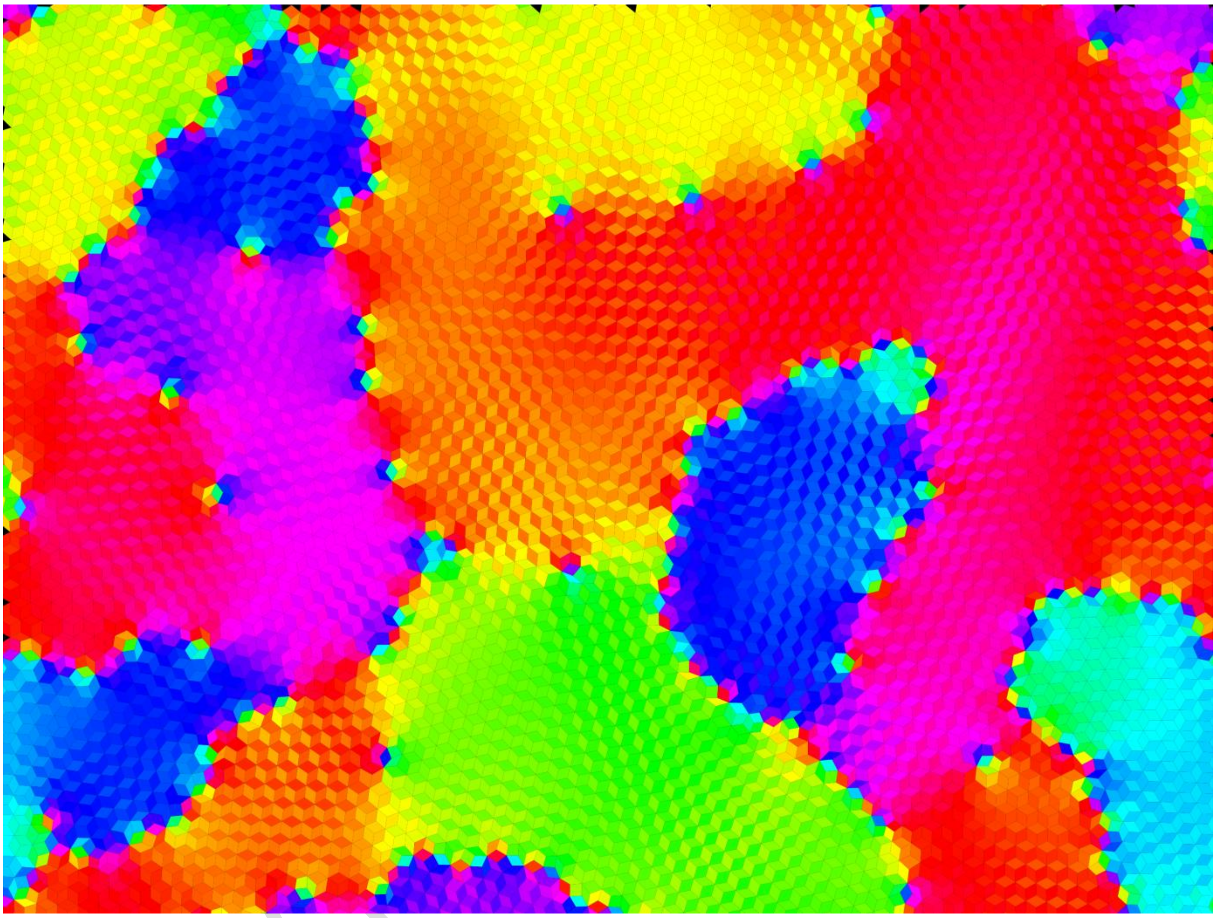
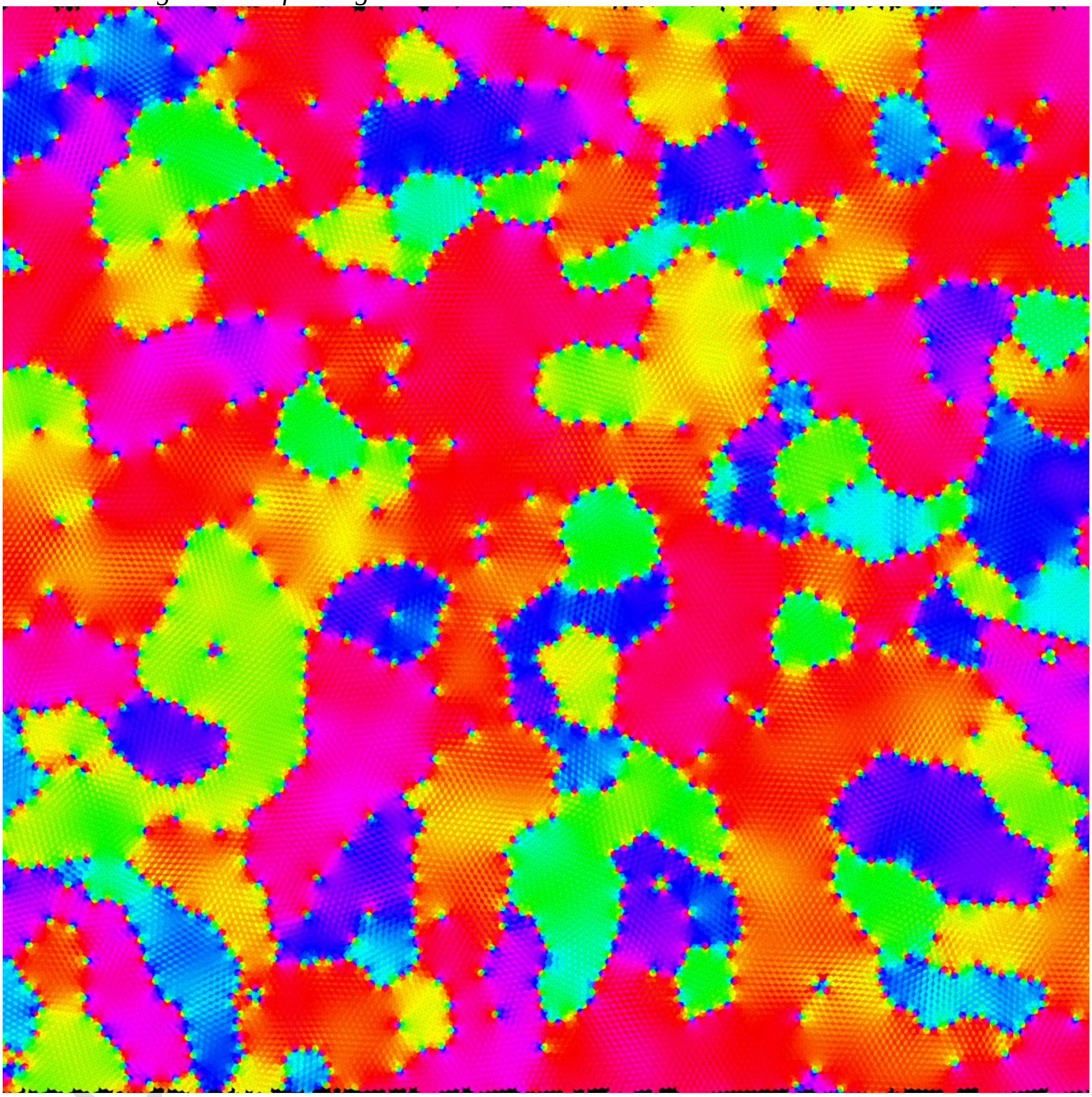


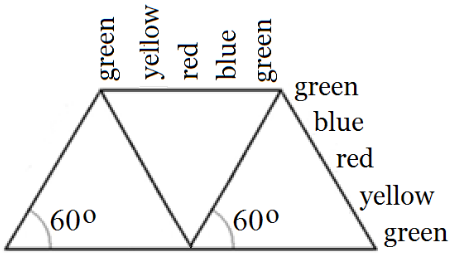
Figure 8. *Another example of crystallization in which each triangle is coloured with the average colour of its edges*



Colour film

Assigning the blue colour to the zero angle, as in Fig. 5, is arbitrary. One can assign, for example, green, Fig. 9, or any other colour as long as one keeps the order of the colours as on the Colour Circle. One can make a movie this way.

Figure 9. *Other than in Fig.5, a way to introduce the colour scale. Direction zero is attributed to green*



The full Colour Circle is divided into N equal parts. Part number n (n = 0, 1, 2, ..., N) is at an angle (n/N) 360º modulo 360º. In the zero (initial) frame of the film, the relationship of colours with directions is as in Fig. 5, (and consequently in Figs. 5 to 8). In n-th frame, the relationship of colours with directions is shifted by (n/N) 360º . If n is even, the colours for n=N/2, are opposite to initial colours for n=0.

General remarks

2D liquid and back to 2D polycrystal

The vibrations of the Voronoi centers soften the structure of the system and lead to the formation of an isotropic 2D liquid. As a result, the grains decease, and disappear. If repeated crystallization is carried out, the more uniform grains are growing, [Lissowski, Wojnar 2001].

Analogue of hexatic phase transition

The hexatic phase is a state of matter that is characterized by a short-range positional In full circle od directions) and a long-range sixfold orientational long order.

The density of pairs 5/7 can be regarded as a measure of an approach to an important hexatic transition, (Nobel 2016).

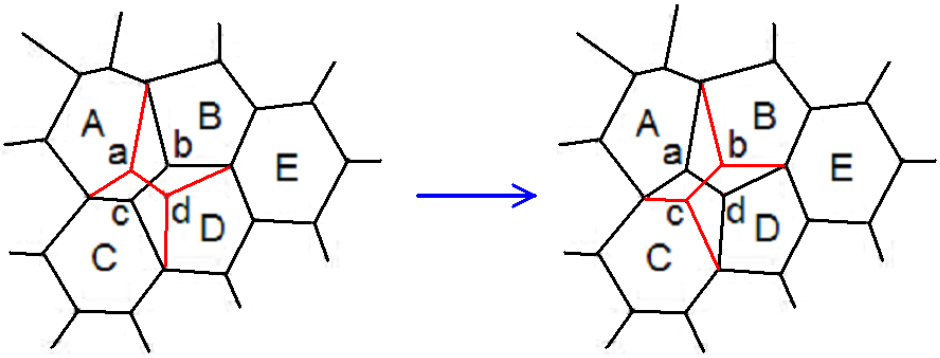
Bragg-Nye's film

The experiment investigates the distribution of soap bubbles on a plane surface. The famous Bragg-Nye's film shows, for example sharp movements of 5/7 pairs created in a 2D bubble polycrystal, and transformations of this polycrystal. For example, single 5/7 long movement could be regarded as a wave-particle duality of a quantum type: the 5/7 dislocation moves on straight lines through the polycrystal while the individual 5/7 bubbles in exchanges of side (flips) only move one step (1/6 of the size of the 5/7 pair).

This phenomenon has a one-dimensional biological analogy in the movement of earthworms. It produces a fold at the end of its body and moves this fold forward. In this way, a small local movement causes the whole body to move forward.

In Fig.10 it is shown dislocation movement as a result of contact change (flip, indicated by red colour). Polygons A and B (penta- and heptagon) in figure at left after exchanging contacts become hexagons in figure at right, and hexagons C and D in figure at left form dislocation pair 5/7 in figure at right.

Figure 10. *Dislocation movement. Contacts exchange of side (bc → ad) and transfer of the 5-7 pair (5/7 dislocation pair: polygons A and B become hexagons, while hexagons C and D create 5/7 dislocation pair*



Packing of cells in epithelial tissue

Epithelium consists of one layer of biological cells.

Francis Lewis noticed that cells in epithelium are arranged in the Voronoi division, [Lewis 1930]. Cell packing in pigmented epithalium of an eye was studied by Lissowski [1970].

Packings 5 and 7 (pentagons and heptagons) of cells and less frequent packings 4 and 8, (quadrilaterals and octagons) or even very rare 3 and 9 (triangles and nonagons) occur in the epithelial tissue, [Rivier, Lissowski 1982].

A comprehensive review of related problems, the Lewis results in particular was given by Edward Bormashenko et al. [2018].

Applications in teaching

The mathematical approach presented in this article should help interested students to familiarize with the concept of crystallization and the packing. It also deals with the foundations of topology, Euler polyhedra, see e.g. Cahn 1970. The method makes it possible to describe numerous natural phenomena, for example, the growth of biological tissues and two-dimensional graphene-type crystals. The quantum wave-particle duality also finds an analogy here.

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