Crystals, Quasicrystals and Shape

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Table of contents

1 Introduction

The question of how crystals grow and are structured has been explored throughout history in many ways. With the discovery of quasicrystals in the mid 1980's some of the assumptions (such as the necessity of translational symmetry-ie. periodicity- and the impossibility of five fold rotational symmetry) have been re-examined. New ways to understand both crystals and quasi crystals have been developed and use various mathematical approaches involving such things as lattices and aperiodic tilings. In their article, "Quasicrystals, Parametric Density, and Wulff-Shape" Borockzy et. al. argue in favor of an approach based on a density function and reliant on the fact that atoms pack more densely if they are arranged in lower energy structures and an understanding of how energy flow acts on boundaries of the crystals.

2 Diffraction Theory

A good place to begin a discussion of crystals is with a short description of diffraction theory. The idea of diffraction theory comes from what happens if you shine light through a grating (for example, a sheet of paper with pin prick holes in some pattern). Light will bend around the edge of the holes in the grating. When this happens one side of the resultant beam of light will lag behind the other side. If the light is all the same wavelength then the peaks of the waves will either add to the intensity of the light (if the waves are in sync) or decrease the intensity of the light (if the peaks are opposing each other. The resultant pattern of light and dark spots can be analyzed to determine the pattern of holes in the grating that was used to create the diffraction pattern. In 1912 it was discovered that crystals could function as diffraction gratings and, furthermore, that the diffraction patterns from crystals could be used to determine the arrangement of atoms in the crystal.

After that researchers assumed that all materials with discrete diffraction patterns would not only display periodicity as well but would also posses only specific rotational symmetries that were compatible with translational periodicity. The discovery in 1982 of materials with supposedly forbidden 5-fold rotational symmetries disproved these assumptions and since that time much work has been done to find unified theories that would serve to elucidate the structure of both crystals and quasicrystals.

First let us begin with a discussion of how crystals are understood.

3 Crystals

Definition 3.1 A crystal is a material that has a discrete diffraction pattern.

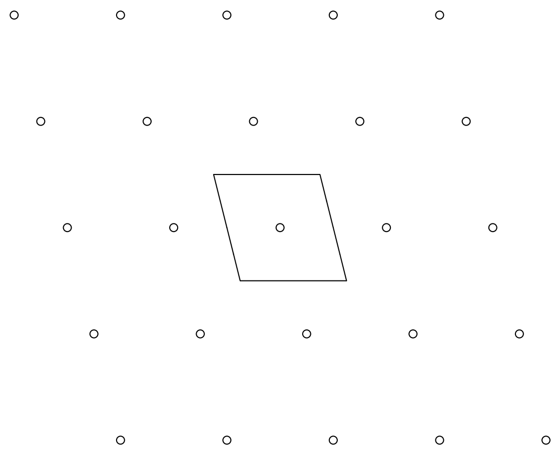
This definition of is relatively new and ultimately resulted from the discovery quasicrystals. It is general so that we can consider quasicrystals a subset of crystals and can deal with them as a special case. A helpful way to think about the atomic structure of any crystal is in terms of a lattice with a delta function at each lattice point. We also want the lattice to have some special characteristics that seem straightforward but should be defined.

Definition 3.2 a set of points Λ is a Delone set if there is some number r such that for every $x, y \in \Lambda, |x-y| \geq 2r$ (ie. it is discrete) and there exists some number R such that every sphere of radius greater than R contains at least one point of Λ (ie it is relatively dense)

A Delone set is, then, a good analogy to the molecules in a crystal. All of the lattices discussed in this paper can be assumed to be Delone sets.

If a crystal posses translational symmetry then the entire lattice can be thought of as a linear combination of a finite set of position vectors. This set of vectors, called a star of the lattice, can be used to recreate the rest of the lattice. The problem is that more than one star can be chosen for a lattice. A better concept to work with is the Voronoi cell.

Definition 3.3 Let Λ be a delone set in n-dimensional Euclidean space (E^n). The voronoi cell of a point x in Λ is the set of all points that are at least as close to x as to any other point in the lattice.



The voronoi cells around the points in the lattice form a tiling of the space.

Definition 3.4 A tiling T of E^n space is a countable collection of closed sets such that $\cup_1^\infty T_i = E^n$ and $\cap_1^\infty T_i = \cup_1^\infty \partial T_i$

4 Parametric Density

Ultimately we want to reach some understanding of the relationship between the order implied by the lattice for the crystal and it's larger order. In other words, how does the configuration of the atoms effect the overall shape of the material. Parametric density can be a first step in understanding this. We can think of the material as being a dense packing of hard balls. In this situation hard balls are balls that do not squish to fill all the space. This will be appropriate for most crystals.

Definition 4.1 Let C_k be the set of vectors $\{c_1, \ldots, c_k\}$ and $convC_k$ be the smallest region that includes C_k (that being a polytope with k vertices). Then Parametric Density for C_k is:

$$\delta = k/(V(convC_k + qB^n)$$

where q is some parameter greater than zero and B^n is an n-dimensional ball with radius 1

Definition 4.2 The determinant of a lattice $detL$ is the smallest region of a lattice such that the entire lattice can be reproduced through translations of $detL$, also called the fundamental domain

When we let the number of vectors increase the parametric density approaches $1/(detL)$.

5 Surface Energy and Wulff Shape

Surface energy describes the energy it takes to maintain an atomic structure. It makes sense to express it as a function of parametric density using the unit vectors u that are orthogonal to the sides of the polytope under consideration as our k vectors.

Definition 5.1 Surface energy for a Polytope P within a lattice L With facets F_i and parameter q¿0

$$E_L(P, q) = \Sigma_i(q - (\delta_L(u_i))/(2 * \delta(L)) \cdot |F_i|$$

Where F_i is the $(n-1)$ "volume" of the facets of P.

The shape that minimizes the surface energy for some lattice is referred to as a Wulff shape.

Definition 5.2 The Wulff Shape for a lattice L with respect to parameter $q > 0$

Wulff shapes found through calculation appear to approximate the actual shapes of the crystals reasonably well.

Example: The natural shape of pyrite is very similar to the Wulff-Shape obtained through calculation

6 Quasicrystals

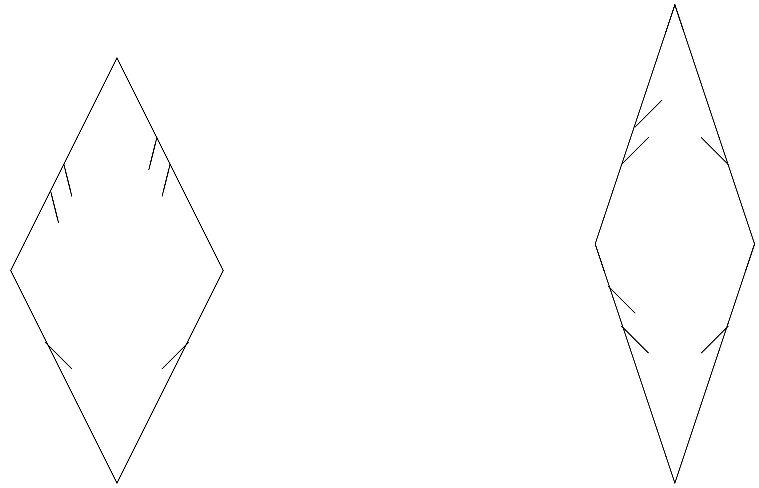
In the mid 1980's researcher began finding materials with discrete diffraction patterns but which did not fit what was believed at the time to be the rules for crystals. The diffraction patterns revealed a lack of translational symmetry and a heretofore assumed impossible five fold rotational symmetry. Up to this point the accepted view was that for there to be long range structure in a material there had to be translational periodicity. But here were materials that disproved that. Much of the research into understanding these quasicrystals began with re-examining a type of tiling found ten years earlier by Roger Penrose.

It's easy to find real world examples of "tilings" that are periodic. For instance, many kitchen floors have square tiles laid out so that the corners of the tiles touch. One can imagine such a tiling continuing infinitely. More difficult to imagine is a non-periodic tiling.

Definition 6.1 A tiling is non-periodic if it admits no translations.

Definition 6.2 A set of tiles is aperiodic if it admits only non-periodic tilings.

Penrose found several aperiodic sets of tiles that provide what we now call Penrose tilings. We want to consider his set of two rhombs. The following figure shows the Penrose rhombs with angles of 2π and 3π for one and π and 5π for the other. The matching rules require that sides only touch if they have the same number of arrows and the arrows go in the same direction.

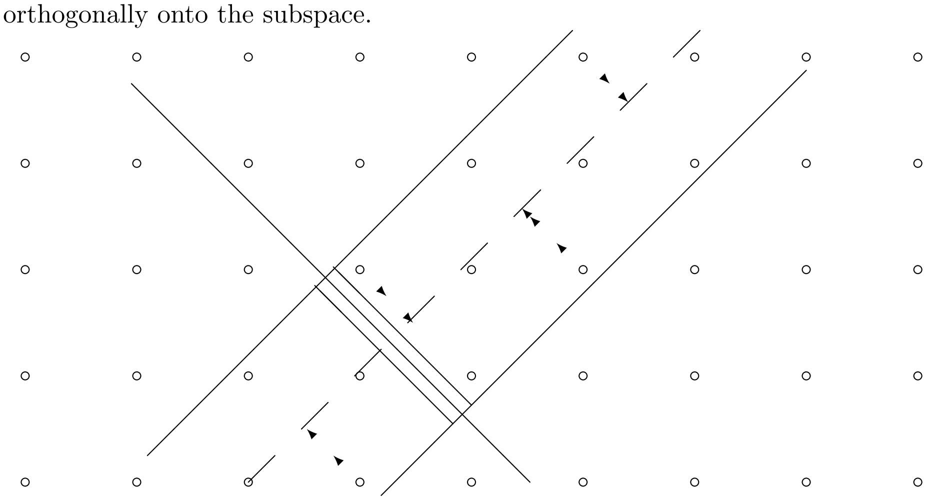


When the matching rules are followed the tilings are forced to be non-periodic. However, they can have the same 5-fold rotational symmetry seen in the diffraction patterns from quasicrystals. One of the ways in which Penrose tilings can be generated is by the project method, also called the cut and project method. First let us introduce a couple concepts.

Definition 6.3 An integer lattice is a lattice in E^n with the lattice points on coordinates with integer values

Definition 6.4 Consider a 2 dimensional integer lattice and consider a line with an irrational slope that passes trough the origin. We call this line an irrational subspace of E^2.

This concept can be generalized to an irrational subspace of higher dimension. Remaining in E^2 for the moment, however, we can easily illustrate the cut and project method. We take a line orthogonal to our subspace and choose a window along this orthogonal line stretching some distance on either side of the subspace. The window gives us a strip along our subspace and we project any points of the lattice that are in that strip orthogonally onto the subspace.



Now we can consider a more complicated situation. Now consider an integer lattice in E^5 with a 2 dimensional subspace. We call the resulting set of points a model set and note that the vertices of a Penrose tiling are an example of a model set conscructed in this manner. At any rate, the pattern is very similar to the diffraction patterns provided by quasicrystals and can tell us about their long range order. Among other things, the similarities between Penrose tilings and quasicrystals can help us define the Wulff-Shape as it pertains to quasicrystals.

Recall that for a regular crystal The Wulff-Shape ultimately depends on the fundamental domain of the lattice. But for a quasicrystal the entire 3 dimensional space is the fundamental domain since there is no translational symmetry. This would make the parametric density equal to zero and that does not work. However the parametric density can be reinterpreted in terms of a subset of a model set.

Definition 6.5 an algebraic extension of L over K is field that is constructed one some base field K and some extension where for every element a in the extension L there exists some nonzero polynomial $p(x)$ with coefficients in K such that $p(a) \neq 0$

An example of this is the field extension of the complex numbers over the real numbers. Every complex number is a root of some non zero polynomial with real coefficients.

Theorem 6.1 let Λ be a primitive model set (ie the projection of L into $E^(n-m)$ is dense) in E^n which can be defined as a basis of the lattice L using an algebraic extension of degree q of the rational numbers. If we have some Jordon measurable subset of an irrational subspace with nonempty interior in E^n and the parameter λ is large then the number of elements in $\lambda K \cap \Lambda$ is

$$card(\lambda K \cap \Lambda) = \delta(\Lambda) V(K) . \lambda^n + O(|lambda^((n-i)/q(n+m))(log\lambda)^(1/q)$$

One model set that meets the conditions for this theorem is the Penrose tiling.

Definition 6.6 A P-set is a union of R Penrose rhombs.

Definition 6.7 $card(P \cap R_k)$ is the number of vertices in a p-set of R rhombs.

7 The Bound of the Area of a P-set

Unfortunately the article by Borockzy et. al. references other articles for proofs of most of it's results. So the following proof was taken from the article, "Quasicrystals and the Wulff-Shape" by Boroczky and Schnell.

Theorem 7.1: let R be a $P-set$. Then

$A(R) \leq sin(\pi/5) * ((\tau+1)/20) * P(R)^2$

with equality if and only if R is the regular decagon. note that $\tau = (\sqrt{5}+1)$

Proof:

Let $x^1, x^2 \in Z^5$such that y^i is the orthogonal projection of x^i onto $\Pi$where Z^5 is the integer lattice in 5 dimensional Euclidean space, $i = 1, 2, \ldots$ are P-points.

Also let $x = x^1 - x^2$, $y = y^1 - y^2$ and the length of an edge of the tiling $l = \sqrt{2/5} * \Sigma_{i=1}^{5} |x_i| = \sqrt{2/5} * ||x||_1$

We want to bound the ratio between $|y|$ and l

We note that $x/||x||_1$ is contained in the polytope defined by $C_r = \{c_1, \ldots, c_r\} \in Z^5$. The projection of C_r onto Π is the regular decagon with circumradius $\sqrt{2/5}$ thus $||(x/||x||_1)|| \leq \sqrt{2/5}$

So $||y||/l = \sqrt{5/2} * ||x/\Pi||/||x||_1 \leq \sqrt{5/2} * ||(||x/x||_1)/(\Pi)|| = \sin(2 * \pi/5)/\sin(2\pi/5 + \alpha) = \cos(\pi/10)/\cos(\pi/10 - \alpha)$

where α is the smallest angle between y and a projection of a unit vector $\pm e_i$.

Let $\beta(y) = \cos(\pi/10)/\cos(\pi/10 - \alpha)$

Then $l \geq \beta(y)/||y||$

If we minimize the value of $\Sigma_{i=1}^{r} \beta(y^i)/||y^i||$ then we maximize the area in the region defined by he vectors y^i.

Let K be a convex polygon with edges $y_1, \ldots, y_r$.

$\tilde{P}(K) = \Sigma_{i=1}^{r} \beta(y^i)/||y^i||$

To minimize $\tilde{P}$ define $W = \cap_{i=1}^{\inf} \{z : w_i z \leq \beta(y_i)$, where $||w_1|| = 1$ and $w_i \perp y_i\}$

There are ten of these $\beta(y_i) = 1$ and these give us a regular decagon.
The article goes on to show (using a lemma from another paper that is not accessible) that

$A(R)/\tilde{P}(K) \leq A(T)/\tilde{P}(T)^2 = A(T)/P(T)^2 = sin(\pi/5) * ((\tau + 1)/20)$

If we let R be a P-set and K be it's convex hull then $A(R) \leq A(K)$ but we also know that $P(R) \geq \tilde{P}(K)$.

Corollary 7.1. Let R be a P-set nd T be the regular decagon. Then

$$\Delta(R, q) \geq \Delta(T, q),$$

with equality if and only if R is T.

8 Conclusion

The article ends with some open questions, the most interesting of which concerns quasicrystals with other rotational symmetries than 5-fold. For instance, quasicrystals have been found with seven fold rotational symmetry. These need cubic extensions instead of quadratic. How is this to be handled? My own questions about this are: how might we construct aperiodic tilings with this symmetry and are there quasicrystals with undiscovered symmetries.

9 Bibliography

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[3] K. Boroczky, Jr., and U. Schnell, *Quasicrystals and the Wulff-Shape*, Discrete Computational Geometry, Vol. 21, 1999, 421–436.