Nanocones: a classification result in chemistry

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Introduction

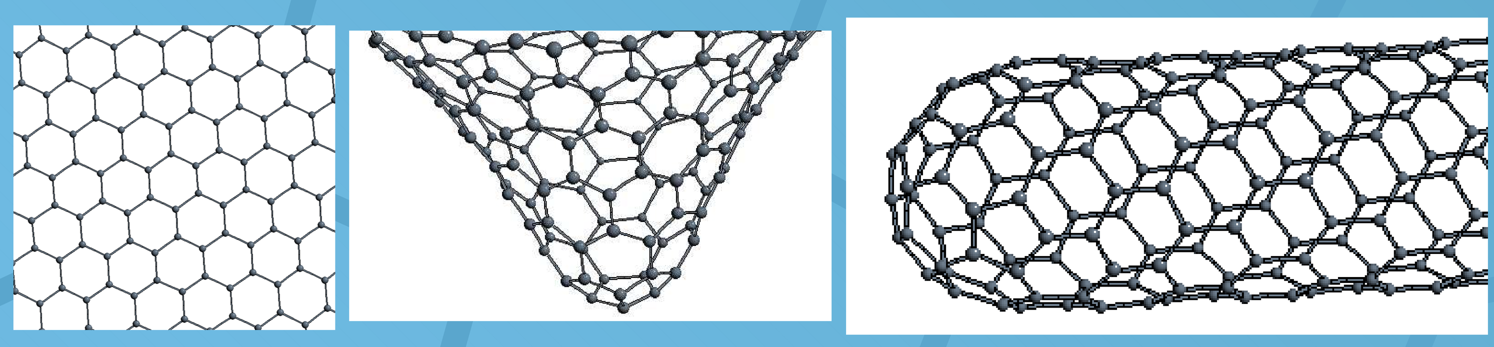


Figure 1: graphite - nanocone - nanotube

Nanocones are carbon networks situated in between graphite and the famous fullerene nanotubes. It is common to all these three that the degree of an atom is 3. Graphite is a planar carbon network where all the faces are hexagons. Fullerene nanotubes are discussed in two forms: once the finite, closed version where except for hexagons you have 12 pentagons and once the one-side infinite version where 6 pentagons bend the molecule so that an infinite tube with constant diameter is formed. A nanocone lies in the middle of graphite and a half-open nanotube: it has between 1 and 5 pentagons besides the hexagons, so that neither the flat shape of graphite nor the constant diameter tube of the nanotubes can be formed. Recently the attention of the chemical world in nanocones has strongly increased. Figure 1 shows an overview of these types of carbon networks.

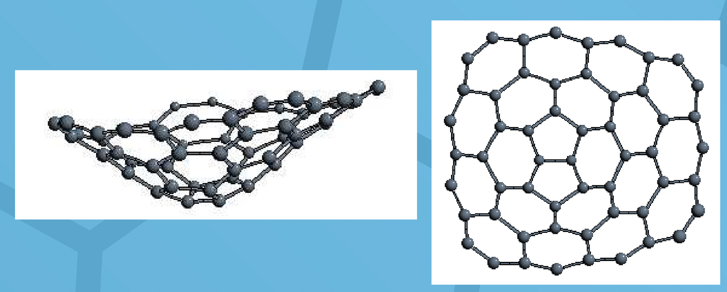


Figure 2: Two views of a patch with two pentagons.

The structure of graphite is uniquely determined, but for nanotubes and nanocones an infinite variety of possibilities exist. There already exist fast algorithms to generate fullerene nanotubes (see [2]) that are e.g. used to detect energetically possible nanotubes, but for nanocones such algorithms don't exist yet.

Goal

To write a generator for nanocones.

Patches

For the generation of these structures we first need to describe an infinite molecule by a unique finite structure from which the cone can be reconstructed. The aim of this poster is to give a rough sketch of this first step. The next step will then be an algorithm to enumerate these finite representations.

A finite and 2-connected piece of a cone that contains all the pentagons is called a patch. All the vertices (atoms) in a cone have degree 3, so the vertices along the boundary of a patch will have degree 2 or 3. It can be easily shown that if the boundary of a patch doesn't contain any consecutive threes, then the number of neigbouring twos is equal to $6-p$, where p is the number of pentagons in the patch.

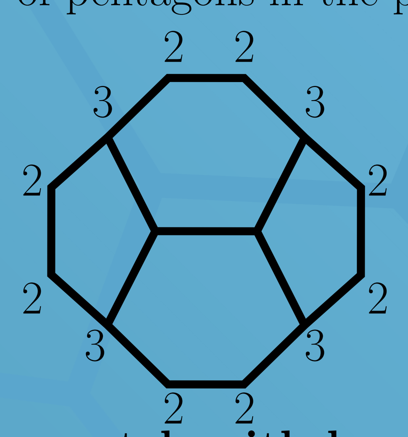


Figure 3: A cone patch with boundary $(2(23)^1)^4$**.**

We can view patches without consecutive threes as polygons where the consecutive twos are the corners, and the lengths of the sides are determined by their number of threes.

Classification

A patch with all sides of equal length is called symmetric and a patch where all except one side are equal and that side is just one shorter is called nearsymmetric.

Theorem

All cones with 1 or 5 pentagons contain a symmetric patch, and all cones with 2, 3 or 4 pentagons contain a symmetric or a nearsymmetric patch.

A similar result was first established in [4]. Here we sketch a shorter proof that can also easily be generalized to other periodic structures.

We interpret a nanocone as a disordered graphite lattice. If you choose a closed path around all disordering pentagons in the cone (described by right and left turns) and then follow the same path in the graphite lattice, then the path isn't closed any more. It can be shown that the starting edge and the final edge can be mapped onto each other by a **symmetry of the lattice** which is in fact a rotation by $p * 60°$. This method to classify disordered patches was invented in [3] and in [1] it was shown that (under the circumstances described here), two disordered tilings are isomorphic – except for a finite region – if and only if these symmetries are the same.

In our case there are only a limited number of possibilities for these symmetries. They are all rotations and are depicted in Table 1. The patches in Table 1 are patches that correspond to these symmetries.

It is easily proven that adding or removing layers of hexagons does not change the type of the boundary.

So together with the theorem of Balke, this proves that all cones are equivalent to one of the cones obtainable from the patches in Table 1.

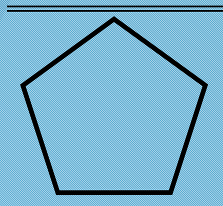
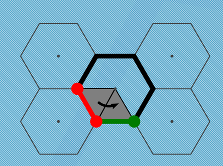
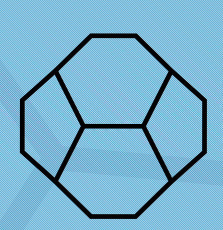
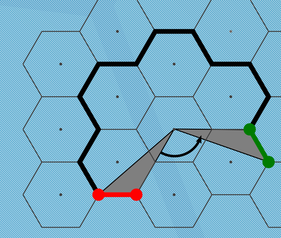
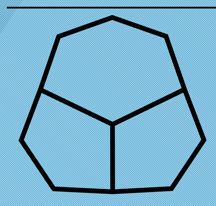
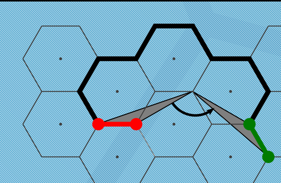
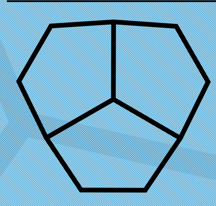
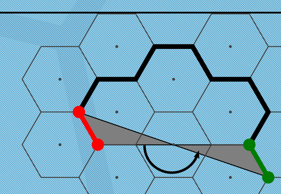
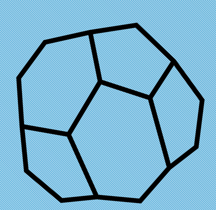
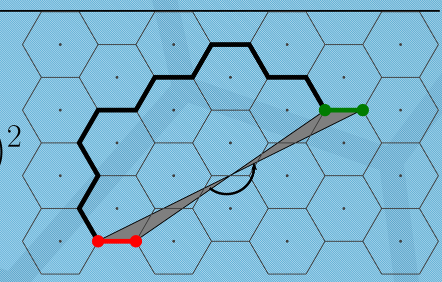
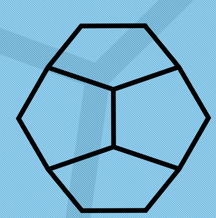
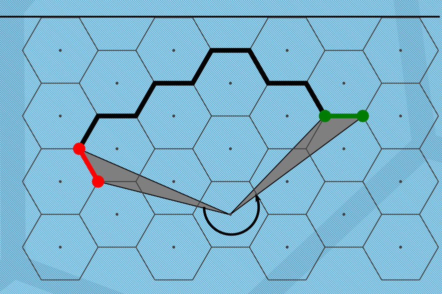
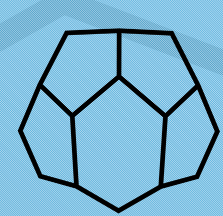
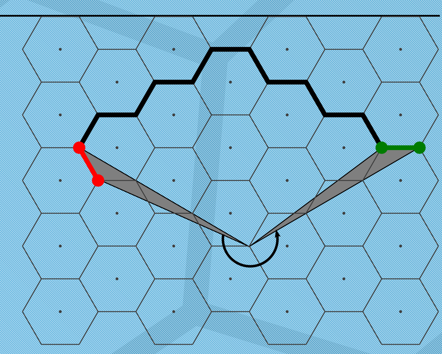
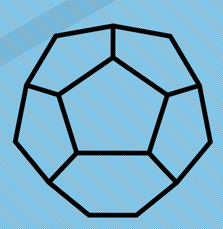
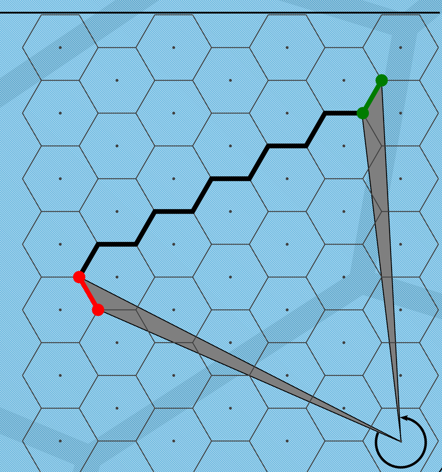
Patch	Boundary	Path
	$2^5 = (2(23)^0)^5$	
	$(2(23)^1)^4$	
	$2(23)^0(2(23)^1)^3$	
	$(2(23)^1)^3$	
	$2(23)^1(2(23)^2)^2$	
	$(2(23)^2)^2$	
	$2(23)^2 2(23)^3$	
	$2(23)^5$	

Table 1: Cones

It also follows from this that no cone contains a symmetric and a nearsymmetric patch, because these boundaries correspond to different automorphisms.

Choosing the boundary that exists due to the theorem in a minimal way leads to a unique patch representing the infinite cone uniquely.

References

[1] L. Balke, *Classification of Disordered Tilings.*, Annals of Combinatorics **1**, 1997, pp.297–311.

[2] G. Brinkmann, U. von Nathusius and A.H.R. Palser, *A constructive enumeration of nanotube caps.*, *Discrete Applied Mathematics* **116**, 2002, pp. 55–71.

[3] A.W.M. Dress, *On the Classification of Local Disorder in Globally Regular Spatial Patterns.*, *Temporal Order, Synergetics 29 Springer*, 1985, pp. 61–66.

[4] D.J. Klein, *Topo-combinatoric categorization of quasi-local graphitic defects.*, Phys. Chem. Chem. Phys. **4**, 2002, pp.2099–2110.

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