NANOCONES
A classification result in chemistry

Gunnar Brinkmann [a], Nico Van Cleemput [a]

[a] *Applied Mathematics and Computer Science, Ghent University, Krijgslaan 281 S9, 9000 Ghent, Belgium*

Key words: Nanocone, Enumeration, Classification

1 Introduction

Nanocones are carbon networks conceptually situated in between graphite and the famous fullerene nanotubes. Graphite is a planar carbon network where each atom has three neighbours and the faces formed are all 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 these: next to hexagons it has between 1 and 5 pentagons, 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.

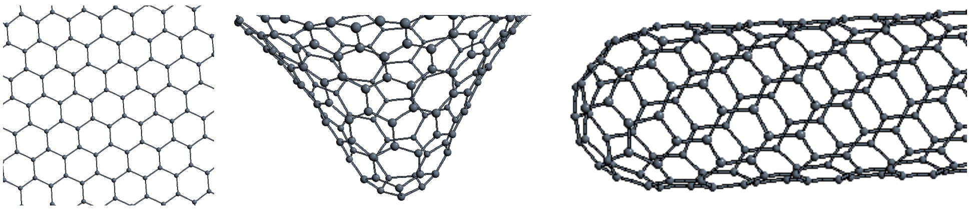


Fig. 1. graphite - nanocone - nanotube

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 [3]) that are e.g. used to detect energetically possible nanotubes. In this talk we describe a generator for nanocones.

Email addresses: `Gunnar.Brinkmann@UGent.be` (Gunnar Brinkmann), `Nicolas.VanCleemput@UGent.be` (Nico Van Cleemput).

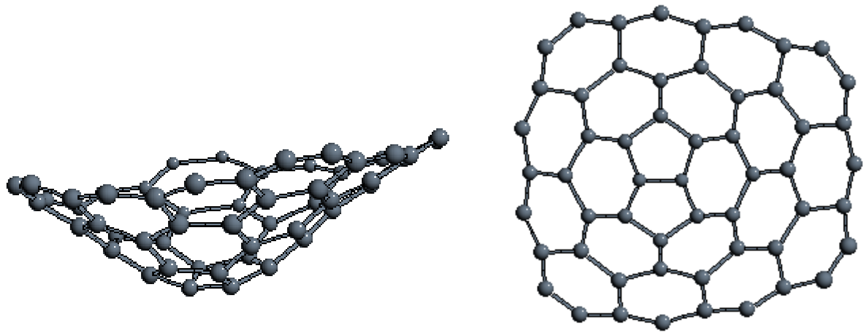


Fig. 2. Two views of a patch with two pentagons.

2 Patches

For computer generation of these structures we first need to describe them in a finite way. We describe the infinite molecule by a unique finite structure from which the cone can be reconstructed. The aim of this talk is to describe this step and give an idea of the algorithm to generate 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.

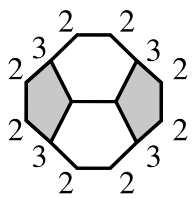


Fig. 3. A cone patch with boundary $(2(23)^1)^4$ and four neighbouring twos.

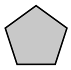
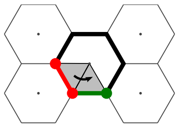
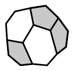
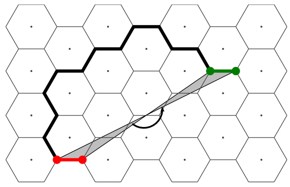
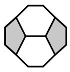
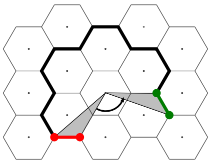
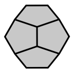
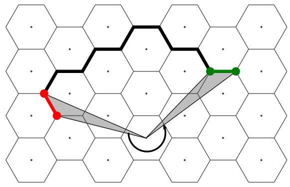
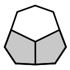
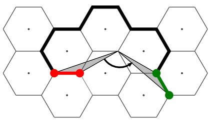
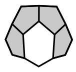
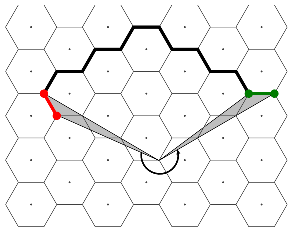
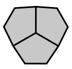
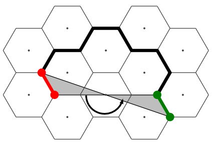
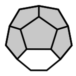
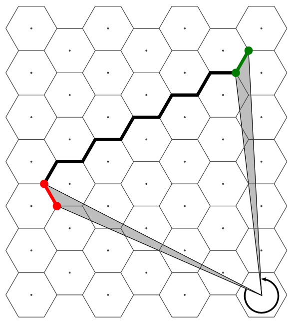
We can interpret patches without consecutive threes as polygons where the consecutive twos are the corners, and the lengths of the sides are determined by their number of threes.

3 Classification

Definition 1 *A* **symmetric patch** *is a patch that has a boundary of the form* $(2(23)^k)^{6-p}$*, with* $1 \leq p \leq 5$*.*
A **nearsymmetric patch** *is a patch that has a boundary of the form* $(2(23)^{k-1})$ $(2(23)^k)^{6-p-1}$*, with* $1 < p < 5$*.*

So in a symmetric patch all sides have an equal length and in a nearsymmetric patch all sides except one have an equal length and that one side is just one shorter than the others.

Table 1: The complete classification of cone patches.

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

Theorem 1 *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.*

This result was first established in [5]. Here we sketch a proof that is not only shorter but can also easily be generalized to other periodic structures.

We interpret a nanocone as a disordered graphite lattice. Choosing a path around all disordering pentagons in the cone (described by right and left turns) and repeating the first edge at the end, and then following this path in the graphite lattice, the first and last edge in the resulting path don't agree anymore. It can be shown that the first edge and the last 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 [4], extended in [2] and in [1] it was shown that (under the circumstances described here), two disorders of the same tiling are isomorphic – except for a finite region – if and only if these symmetries are equivalent. Two

rotations are said to be equivalent when they rotate among the same angle, and the centers of rotation are equivalent under a symmetry of the tiling.
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, i.e. whether the boundary is symmetric or nearsymmetric.
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.
It also follows from Table 1 that no cone contains a symmetric and a nearsymmetric patch which both contain all the pentagons in the cone, because such boundaries correspond to different automorphisms.
Choosing the boundary that exists due to Theorem 1 in a shortest way leads to a unique patch that fully describes the nanocone.

In fact this classification even leads to a unique patch, so we have the following theorem.

Theorem 2 *There is a 1-1 correspondence between the set of symmetric and nearsymmetric patches and the set of nanocones.*

An algorithm to generate these patches will be sketched in the talk. It was implemented and tested against an independent algorithm to verify the results.

References

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

[2] G. Brinkmann, *Zur mathematischen Behandlung gestörter Pflasterungen*, Ph.D. thesis, University of Bielefeld, 1990.

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

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

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