Short communication

Art and Science: Geodesy in Materials Science

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This paper is dedicated to Professor Milan Randić on the occasion of his 80th birthday

Abstract

A 3-dimensional model based on a molecular structural recipe having some unique and unexpected shape characteristics is demonstrated. The project was originally initiated to satisfy the aesthetic creative impulse to build a 3-dimensional model or sculpture. Further scientific investigation explained some important nanoscale structural observations that had been seen many years beforehand and mistakenly explained. This is a rare example of artistic creativity resulting in a key scientific advance.

Keywords: Material Science, Giant Fullerene model, nanoscale structure, quasi icosahedral shape

1. Introduction

In 1988 Ken McKay and I carried out a fascinating little project primarily for fun which inadvertently made a major contribution to our understanding of carbon particles whose structures at nanoscale dimensions had heretofore been impossible to understand although several attempts had been made over many years resulting in quite erroneous conclusions which had been accepted for several decades.[1]

1. 2. Geodesic Domes

After the Fullerenes had been discovered[2] I thought, in the late 1980s, it might be neat to build my own mini-Buckminster Fuller Dome (like the one pictured in Fig 1 but a little smaller!) and purchased molecular modelling kits to do it. There was no thought at the time that this was a research project – it was just a fun project to build a large beautiful model to display essentially like a sculpture in our laboratory. The image of Buckminster Fuller's famous Dome at the Montreal Expo 1967 shown in Fig 1 is from Graphis 1967.

Figure 1. Photograph of the Buckminster Fuller's Dome at the Montreal Expo 1967.

The original little fun project with Ken McKay led us first to some fascinating work by the mathematicians Goldberg and Coxeter on what are now called Goldberg polyhedra. When the models were constructed, much to

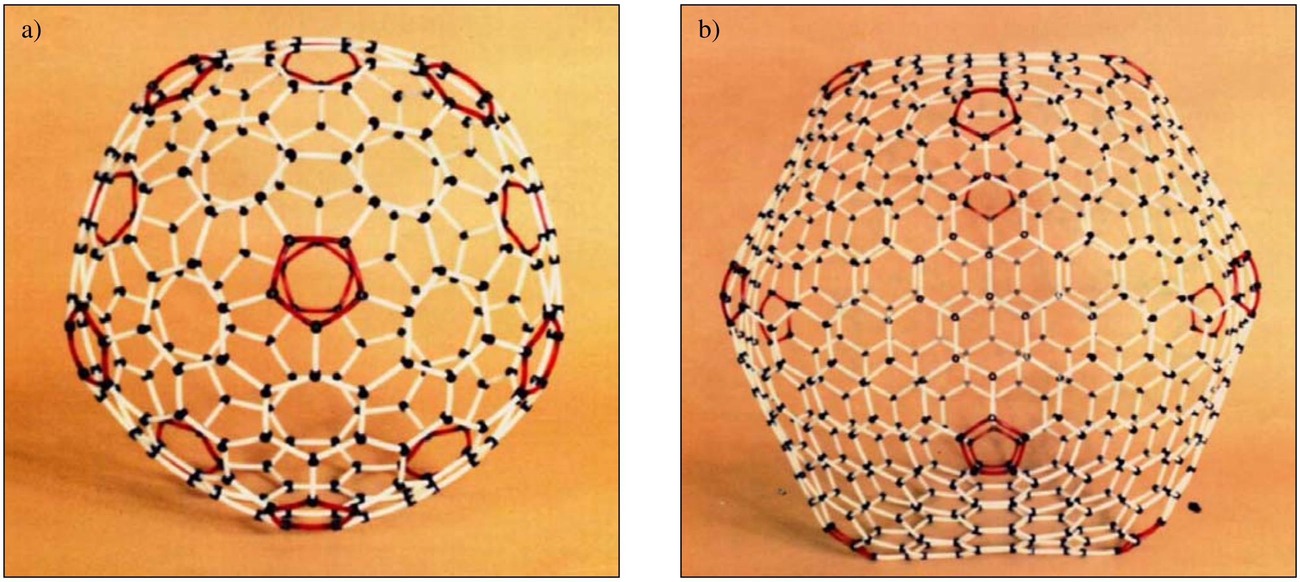
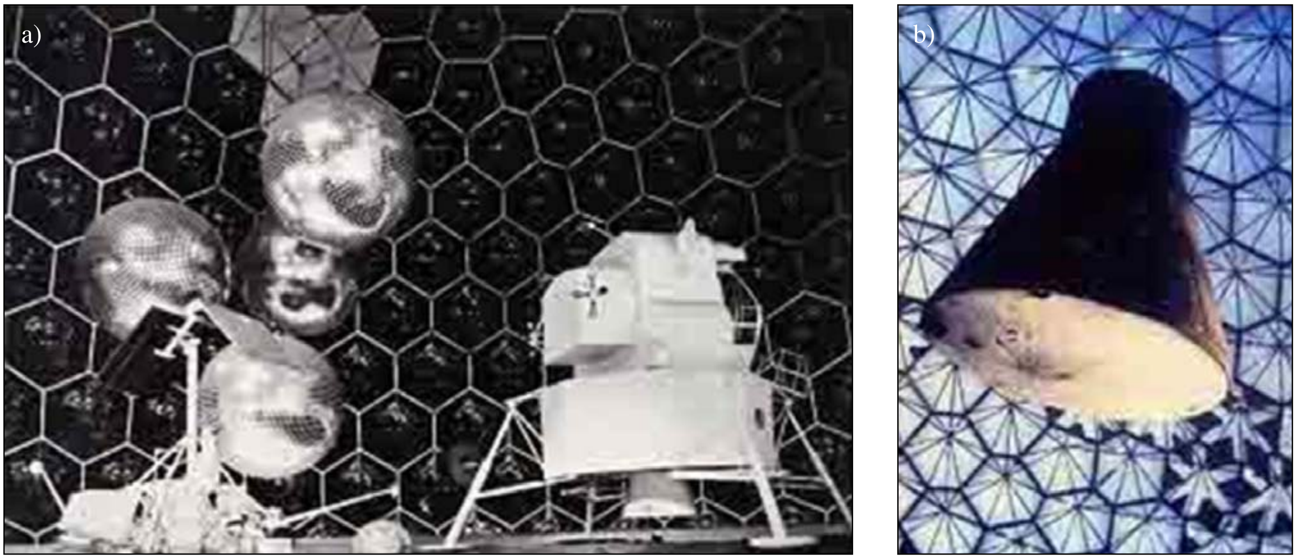


Figure 2. Photographs of molecular models of the Giant Fullerenes C_{540} (a) and C_{960} (b). The models were based on the Goldberg polyhedra. Notice that as the cages become larger the icosahedral symmetry of the structure becomes more and more obvious as the overall shape becomes less spheroidal and more polyhedral.

my surprise they were not smoothly spherical like the dome above. I had assumed this would be the case from my cursory perusal of the images of all the domes I had seen. Instead each model that we constructed (cf Fig 2a and Fig 2b) was essentially a closed icosahedral monosurface consisting of a hexagonal network of struts that swept from one, of 12, pentagonal cusps to another.

I remember being quite perplexed at the time as to why the models were not spheroidal as I had expected. Then I returned to study images of Fuller's domes much more carefully and realised that although the hexagons were in general fairly symmetric those in the neighbourhood of the pentagons were quite distorted as can be seen in Fig 3.

Then I realised that I (and apparently everyone else) had overlooked something that had been under our noses in the literature for years. I had looked at electron microscope images of spheroidal carbon particles several times



Figures 3. Two images taken from inside the Expo 67 Dome. The left hand photograph (a) was published in Graphis 43 (1967) and the right hand one (b) was taken by Robin Whyman who kindly gave me a copy of his slide. By great good fortune these photographs which are of the first US space capsule and an Eagle Moon Lander replica also both show a pentagon. Particularly interesting from the science/art point of view is the asymmetry of the hexagons which abut the pentagons. This distortion was necessary to produce the near spheroidal structure of the Expo 67 Dome. The Giant Fullerenes possess their own unique quasi-icosahedral "Giant Fullerene" shapes consisting of relatively smooth surfaces which sweep between the 12 pentagonal cusps necessary for closure of each Fullerene.

in the past and only now realised what I must have been looking at. Several years earlier high resolution electron microscope images of onion-like structures (cf Iijima 1980) had been published. A typical example of these elegant images is shown in Fig 7 where a picture taken by Daniel Ugarte is depicted. The electron microscope yields an image that can be considered as a sort of cross-section of the spheroidal particle that actually consists of concentric spheroidal shells, much like an onion. Thus one can effectively get an image of the structure that one has effectively sliced into two hemispheres to reveal the inner structure, much as cutting horizontally through a tree trunk reveals tree rings. What I realised was that I and others had missed the fact that the rings were not quite circular but possessed subtle curvature variations which betrayed the fact that they were actually quasi icosahedral as were our Giant Fullerene models. I had seen what I wanted to see rather than what was actually there. To find quantitative confirmation of this conjecture Ken wrote a computer programmes to create a set of Giant Fullerenes of ever increasing size Fig 4.

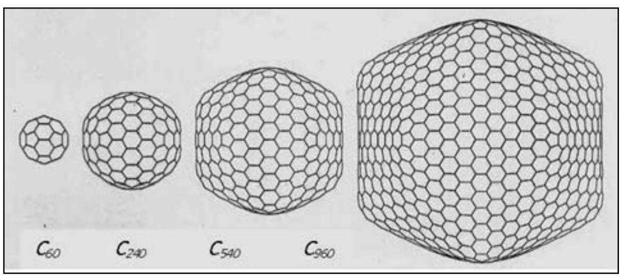


Figure 4. Set of Giant Fullerenes of gradually increasing size.

The cages were then placed one inside the other as shown in Fig 5.

In an electron microscope a beam of electrons is passed through an object and if the beam encounters an array of atoms which possess some phase relation as they do when the electrons pass along a channel in which a graphite wall lies, then the atoms may be diffracted and a dark line appears in the resulting pattern cf Fig 6 a and b. One then observes what is effectively a cross section of the particle. The Fullerenes tend to show polygons with something between 6 fold and 10 fold symmetry. Of course perfect icosahedral symmetry is very unlikely but flattening should be, and is, quite common Fig 7 and Fig 8.

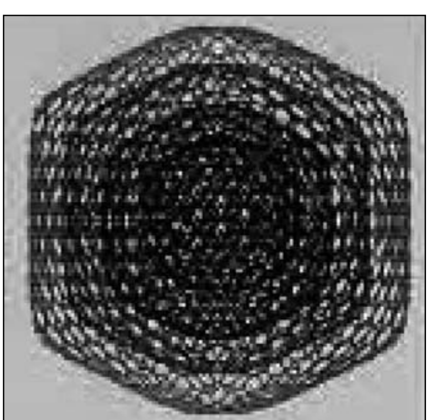


Figure 5. Schematic diagram depicting four Fullerene Cages in an onion-like concentric arrangement.

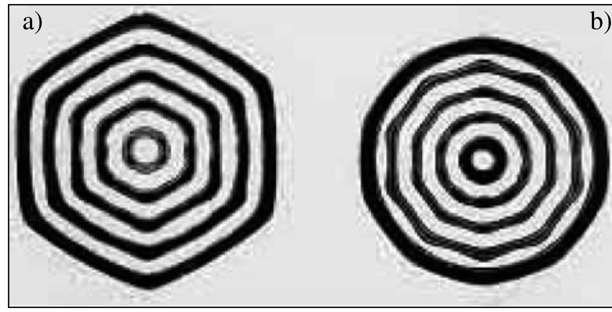


Figure 6. Simulated high resolution electron microscope images of a carbon particle consisting of 5 concentric Fullerene cages seen along two different axes; a) The left hand image shows 6-fold symmetry whereas b) the right hand image shows 10-fold symmetry.

Figure 7. Actual high resolution electron microscope image of an onion-like spheroidal carbon particle. Flattening of the shells is most obvious in the arcs between 8 o'clock and 11 o'clock. Image from Daniel Ugarte.

2. Conclusion

In this paper an account is given of a project which was originally initiated to satisfy the aesthetic creative impulse to build a 3-dimensional model or sculpture based on a molecular structural recipe. In the event the resulting model turned out to have some unique and unexpected shape characteristics which led to further scientific investigation that explained some important nanoscale structu-

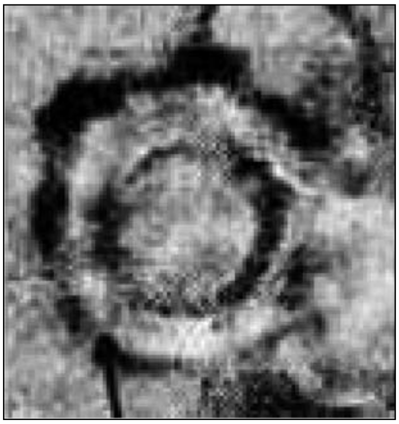


Figure 8. Actual high resolution electron microscope spheroidal carbon particle consisting of only two shells. The hexagonal shape of the outer shell is very clear and is totally consistent with the simulation shown in Fig 6. (Image from Mordkovich and Endo).

ral observations that had been seen may years beforehand and mistakenly explained. The account is a rare example of artistic creativity resulting in a key scientific advance.

3. Acknowledgements

I wish to thank Ken McKay and David Wales my colleagues in the original scientific investigation and Daniel Ugarte and Morinobu Endo for their electron microscope their images.

4. References

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Povzetek

Prikazan je 3-dimenzionalni model, ki temelji na zakonitostih molekulske strukture in ima nekatere edinstvene in nepričakovane lastnosti, ki vplivajo na obliko. Projekt je bil v začetku namenjen za uresničevanje kreativnih estetskih idej za izgradnjo 3-dimenzionalnega modela ali skulpture. Nadaljnje znanstvene raziskave so pojasnile nekaj pomembnih opažanj na nivoju nanostruktur, ki so bile mnogo pred časom in napačno razumljene. To je redek primer umetniške kreativnosti, ki je bistveno vplivala na napredek znanosti.