

## CONSTRUCTION OF A MECHANICAL MODEL FOR THE EXPANSION OF A VIRUS

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### Abstract

Many viruses have an outer protein coat with the structure of a truncated icosahedron, and can expand following changes to the environment around the virus. The protein coat consists of chemically identical protein subunits that form pentagonal or hexagonal capsomeres; these move apart during expansion, opening interstices and allowing access to the interior of the virus coat. A virus whose expansion has been well characterised is the cowpea chlorotic mottle virus (CCMV). Detailed observation of the CCMV shows that the connection between capsomeres consists of a double-link with local  $C_2$  symmetry. The present paper describes the construction of a simple physical model of the CCMV; it consists of rigid pentagonal and hexagonal plates modelling the capsomeres, connected by spherically jointed bars that preserves the double link nature of the connection between capsomeres. Analysis has shown that this model is guaranteed to have a totally symmetric swelling mode — this expansion mode of the physical model reproduces the key characteristics of the expansion of the CCMV.

### 1 Introduction

Many viruses consist of an outer protein coat (the virion) containing a DNA or RNA ‘payload’, where the virion undergoes reversible structural changes that allow switchable access to the interior by the opening of interstices through expansion. These changes may be driven, for example, by variations in pH of the biological medium. The present paper introduces a mechanical model that helps to explain the expansion of the virion in terms of classical principles of structural mechanics.

An expanding virus that has been well characterised is the cowpea chlorotic mottle virus (CCMV), shown in Figure 1, which has a structure based on the truncated icosahedron ( $T = 3$  in the standard notation for triangulated icosahedral structures ([CAS62])). In the native form, stable around pH 5, 180 chemically identical protein subunits form a shell of diameter  $\simeq 286$  Å. The protein subunits form into either pentagonal or hexagonal capsomeres. At pH 7, the virus particles undergo a 10% increase in radius, thought to occur as a result of deprotonation of carboxyl moieties at the inter-capsomere contacts, leading to electrostatic repulsion that opens out the structure, but the process falls short of complete disassembly through preservation of interwoven carboxyl/protein links between capsomeres ([SPE95]). Discrete swollen states have also been observed in many plant viruses, e.g. turnip crinkle ([SOR86]), tomato bushy stunt ([ROB82]) and southern bean mosaic viruses ([RAY79]), and similar phenomena have been inferred for animal viruses such as poliovirus ([FRI90]). An important feature of the swelling process is that it leads to opening of a 20 Å-diameter portal on the quasi-threefold axes at full expansion. Exploitation of these portals for pH-gated material transport and fabrication of mineralised nanoparticles has been proposed ([DOU98], [DOU99]).

Detailed observation of the CCMV shows that the connection between capsomeres consists of a double-link with local  $C_2$  symmetry. Based on this, Kovács *et al.* ([KOV04]) have introduced a class of expandable polyhedral structures, the *double-link expandohedra*. The present paper describes the construction of a physical model of a double-link expandohedron that provides a simplified mechanical model for the expansion of the CCMV.

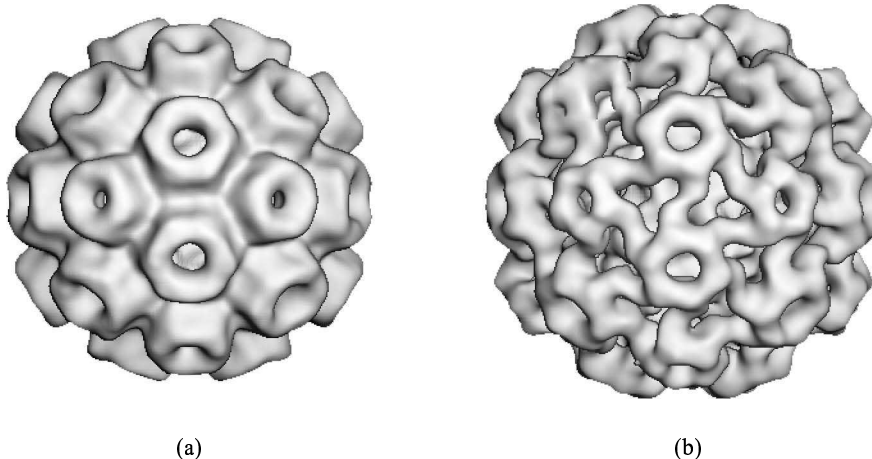


Figure 1: Cryoelectron microscopy and image reconstruction of the cowpea chlorotic mottle virus (CCMV): (a) in an unswollen condition compatible with low pH; (b) in a swollen condition induced by high pH. Note that the capsomeres are either hexagonal or pentagonal, arranged in the  $T = 3$  pattern of a truncated icosahedron. Detailed study shows that the connection between capsomeres is formed by a double protein link that is not resolved in these images. Images provided by T. Baker, Purdue University.

## 2 Double-link expandohedra

In the present paper, we are particularly interested in the double-link expandohedron based on the  $T = 3$  icosahedral structure of a truncated icosahedron; however, in general, a double-link expandohedron can be constructed from any trivalent polyhedral parent. The construction is as follows. First the faces of the parent polyhedron are separated to give a distinct rigid prism for each face, the same in size and shape as the original. These rigid face prisms are then linked by a pair of bars that are connected to the prisms by spherical joints: these bars run ‘diagonally’ across the gap. The choice of sense of diagonals is made cyclically on some starting face, and then propagated consistently over the whole set of face prisms. Figure 2 shows a possible arrangement of bars around a regular pentagonal face, where each bar runs from one vertex to the mid-point of an adjacent side.

The construction described gives a ‘fully closed’ configuration, where the bars along an edge are both co-linear with that edge. However, a more general initial geometric configuration would be given by initially displacing the face prisms in some way consistent with the symmetry of the original polyhedral parent, and then generating the bars. There is a great deal of latitude in the placement of the bars. In CCMV for example, the linking protein strands, modelled here by spherically-jointed bars, are anchored *within* the capsomere subunits. The only conditions that the bar placement *must* follow are that the disposition of the bars should respect any rotational symmetries of parent polyhedron, and the bars must not coincide.

The possible motion of a double-link expandohedron can be initially explored using the mobility criterion, a simple generic counting relationship for calculating the degrees of freedom of a mechanical linkage ([HUN78]). In a form that allows for non-independent constraints ([GUE04]) the mobility of a linkage consisting of  $n$  bodies connected by  $g$  joints, where joint  $i$  provides  $c_i$  constraints, is given by

$$m - s = 6(n - 1) - \sum_{i=1}^g c_i, \quad (1)$$

where  $m$  is the number of mechanisms and  $s$  is the number of states of self-stress that the linkage can sustain (a state of self-stress is a set of internal forces in the linkage in equilibrium with zero external load).

For the double-link expandohedron, we consider each face as a rigid body; the double link between faces is then considered as a pair of length constraints. For the double-link expandohedron

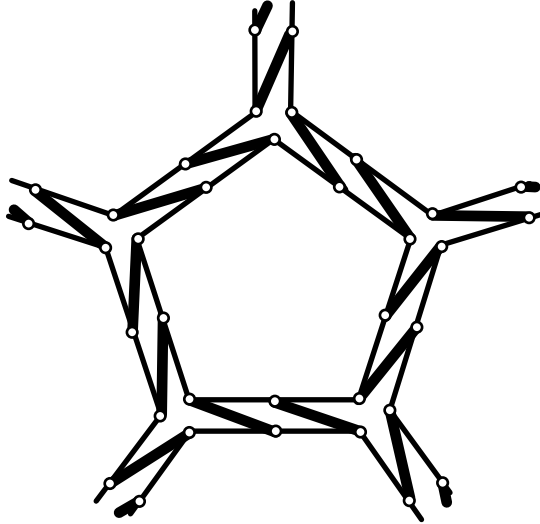


Figure 2: The construction of a double-link expandedhedron around a regular pentagonal face. A simple arrangement, in which links run from vertices to edge mid-points, is shown; many other arrangements are compatible with the construction described in the text.

based on the truncated icosahedron that is of interest here, there are 32 faces (12 pentagons and 20 hexagons), and hence  $n = 32$ . There are 90 edges, each providing two constraints, and hence  $g = 90$  and  $c_i = 2$ . Thus

$$m - s = 6 \times (32 - 1) - 2 \times 90 = 6, \quad (2)$$

and, in fact, it is straightforward to show that this is true for a double-link expandedhedron based on any trivalent parent polyhedron.

Thus, the double-link expandedhedron model of the CCMV has at least six mechanisms, but simple counting gives no information about the nature of these mechanisms; they may be finite or infinitesimal, and may or may not include a fully symmetric breathing mode. However, a symmetry analysis, described by Kovács *et al.* ([KOV04]) using a symmetry extension of the mobility rule ([GUE04]) helps to clarify these issues. This shows that, for the  $T = 3$  icosahedral double-link expandedhedron in a generic configuration, there are in fact  $m = 9$  mechanisms, and  $s = 3$  states of self-stress (consistent with Eq. (2)). Further, it is shown that one of the mechanisms is totally symmetric, without a corresponding equisymmetric state of self-stress, and this is enough to guarantee that this mechanism must be a finite mechanism ([KAN99]). Thus, the mechanical model described in this paper is *guaranteed* to have a swelling mode, to model the expansion of the CCMV.

### 3 The Mechanical Model

This section describes a physical model of the  $T = 3$  icosahedral structure that we have constructed. When fully closed this model has the appearance of a truncated icosahedron; hidden behind each edge is a pair of linking bars connecting adjacent faces.

The mechanical model consists of 20 hexagonal plates, and 12 pentagonal plates. They each have a side length of 50 mm, and were cut from 0.9 mm thick aluminium alloy sheet with a spark-eroding wire cutter. Close to each edge of the plates two 2 mm holes were drilled, where the link bars were to be fitted. The link bars between faces consist of stainless steel hypodermic needle of length 20 mm and diameter 2.6 mm. A piece of elasticated string is stretched through this hollow cylinder. At each end the elastic string passes through a hole in one of the polyhedral plates; it is then locked off in a slot cut into the edge of the plate. A schematic view of a single link is shown in Figure 3; Figure 4 show an actual double link from the final model, formed between a hexagonal and a pentagonal plate.

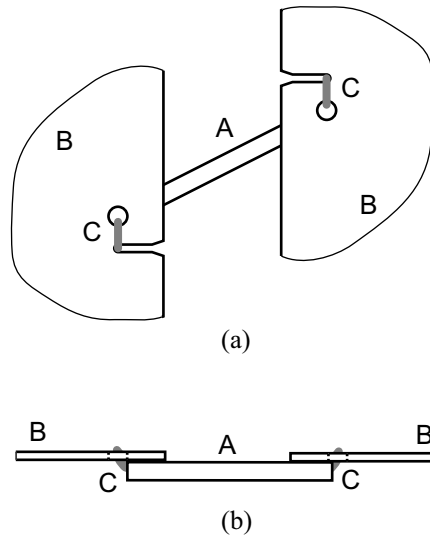


Figure 3: A schematic view of a single link: (a) plan view, from ‘outside’ the model; (b) elevation. The link A consists of a hypodermic needle linking two plates B. A piece of elastic string C passes through the hypodermic needle and through holes in the plate, and is locked off in slots cut into the edge of the plates.

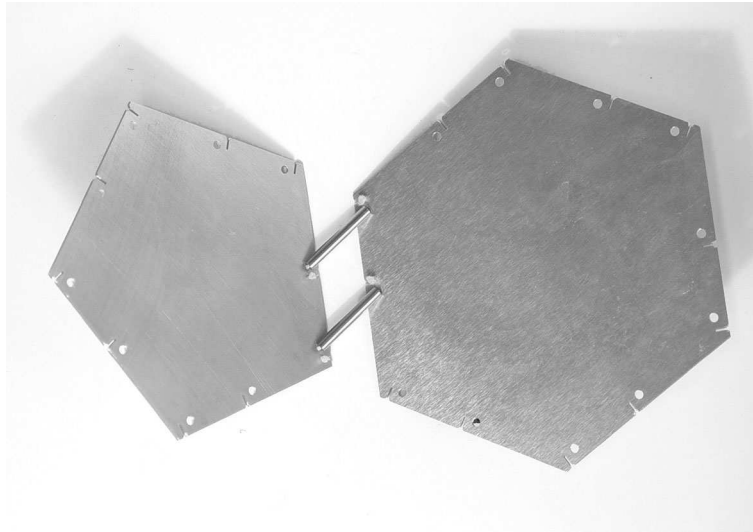


Figure 4: The double-link between a pentagonal plate, and a hexagonal plate, shown from the ‘inside’ of the model. Each link consists of a length of hypodermic needle connecting pairs of holes in the plates; a length of elastic string passes through the hypodermic needle and the holes, and is locked off in a slot cut into the edge of the plates.

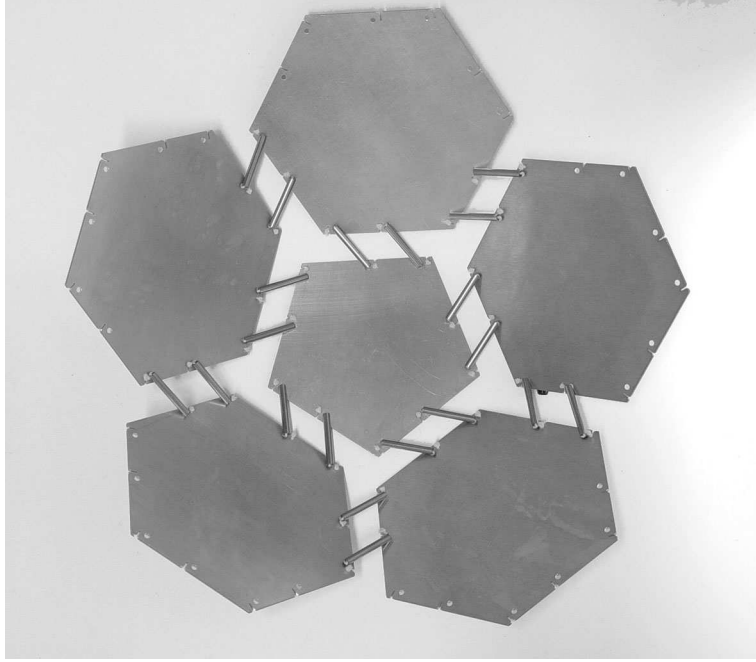


Figure 5: A complete set of links surrounding a pentagonal plate, shown from ‘inside’ the model.

The links between plates are repeated cyclically around the faces of the truncated icosahedron; Figure 5 shows the complete set of links around one of the pentagonal plates. The construction of the model, with links connected by elasticated string, leads to the relaxed form of the links being in the open configuration shown.

The final model of the  $T = 3$  icosahedral double-link expandohedron is shown, in both open and closed forms, in Figure 6. In the closed form, the plates that represent the capsomeres of the CCMV fit together to give a truncated icosahedron; the linking bars are hidden behind the edges of the polyhedron. Opening the model destroys the apparent reflection symmetry, but preserves the rotation symmetry of the icosahedron to give a chiral form of the structure. The relaxed form of the model is in the open configuration. To hold it in the closed configuration shown in Figure 6, short lengths of adhesive tape were added around each trivalent vertex of the truncated icosahedron; these connections model the carboxyl links that keep the CCMV in its closed configuration in a low pH environment.

A comparison of Figures 1 and 6 shows that the mechanical model of the double-link expandohedron captures the basic swelling mode of the CCMV. One interesting distinction is that, for the CCMV, the pentagonal capsomeres expand by less than the hexagonal capsomeres, leading to a dimpled appearance; this does not occur for the mechanical model. However, it is clear from the model that the geometry of the links would allow each pentagonal face to be ‘popped-through’ separately into a dimpled form, although in the actual model, physical interference between the links and the pentagonal plate prevents this.

#### 4 Conclusions

The model as constructed has confirmed the analytical and numerical results in Kovacs et al. ([KOV04]), which predicted that a double-link expandohedron would have a totally symmetric ‘breathing’ mode that corresponds to the expansion of the CCMV.

In building this model, no attempt has been made to generate a correct link geometry that models in exact detail the expansion of the CCMV; the actual end points of the linking bars for the CCMV appear to be further away from the edge of the capsomeres than shown in our model. However, it would be straightforward to construct a more accurate model of the CCMV using essentially similar construction techniques.

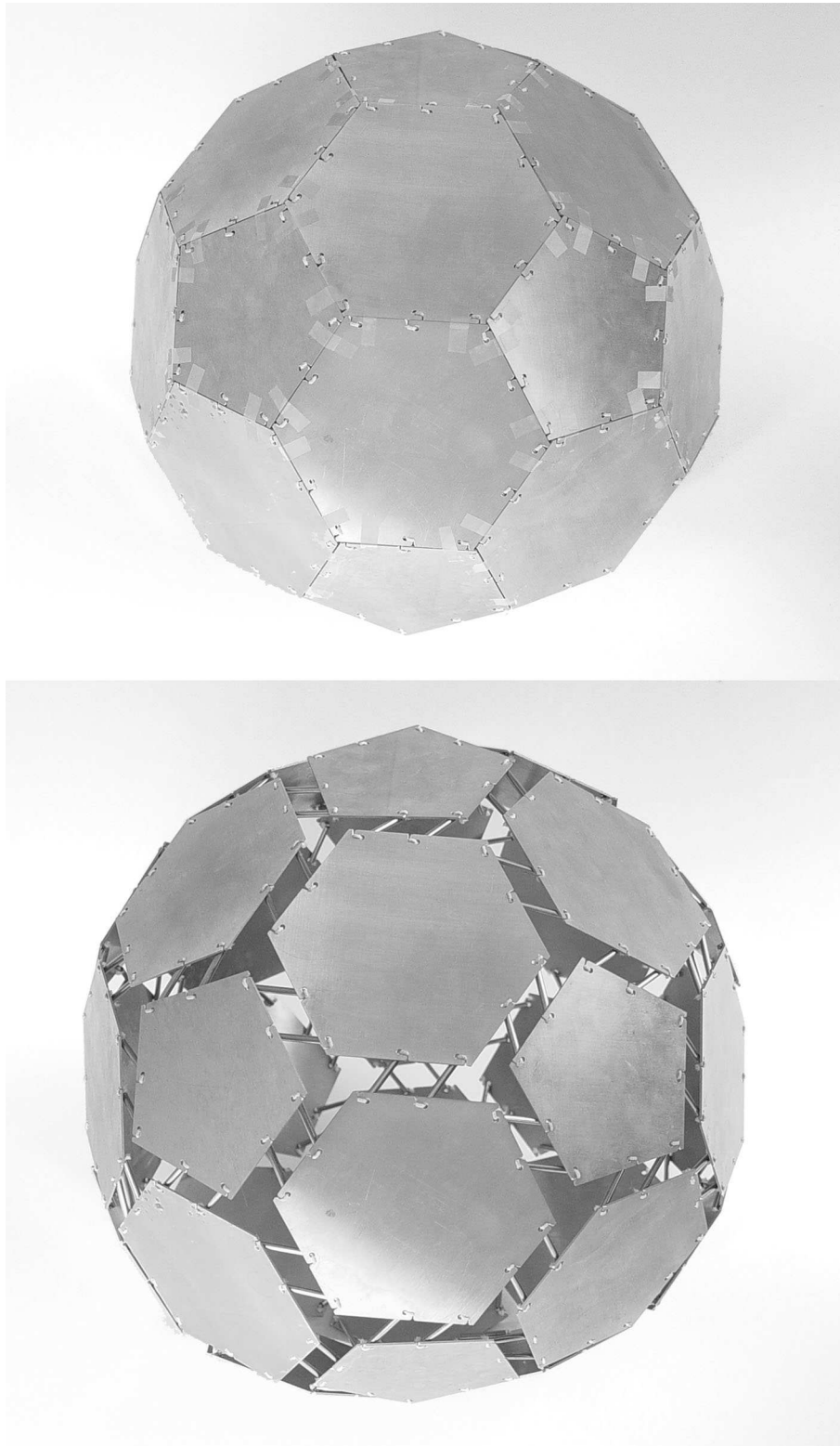


Figure 6: The final model, shown open and closed. Due to the method of link construction, the open state is the relaxed state. In the closed configuration, the faces are held together by adhesive tape, modelling the carboxyl links between capsomeres in the CCMV

An interesting observation that has emerged from building  $T = 3$  icosahedral double-link expandohedron models is that there is not a unique swollen configuration of the structure; each pentagonal face seems able to assume either a proud, or a dimpled, configuration, although moving a pentagonal face from one state to the other requires deformation of the structure, leading to a snap-through phenomenon. Further research is required to elucidate the unfolding paths that may lead to these configurations, and the connection with the geometry of the links in the CCMV that leads to a dimpled configuration.

A drawback of the construction of the model described in this paper is that the links prove to be rather fragile, and wear easily at the intersection of the linking bar and the plate. To make future models more robust, it will be necessary to design this detail more carefully.

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