Viral capsids and self assembly
Viral capsids

helical symmetry

Capsid

RNA

protein subunit

capsid proteins are wrapped around the viral RNA
(e.g. Tobacco Mosaic Virus)

icosahedral symmetry

Hepatitis B virus

conical shaped
(spherical caps usually still icosahedral)

complex symmetry

Poxvirus

Note: many viruses also have envelope (lipid bilayer) around the capsid

HIV
Icosahedral capsids

Brome mosaic virus

L-A virus

Bacteriophage \(\phi X\) 174

Cowpea Chlorotic Mottle virus

Dengue virus

Tobacco Necrosis virus

Human Hepatitis B Virus

Sindbis virus

Bacteriophage HK97

Simian virus

Colors correspond to different proteins.
Caspar-Klug classification of icosahedral capsids

Generating vector

\[ \vec{A} = h\vec{a}_1 + k\vec{a}_2 \]

Icosahedral frame on a hexagonal lattice (h=1,k=2)

\[ T = \vec{A}^2 = h^2 + k^2 + hk \]

12 pentamers (vertices of icosahedron)
10 (T-1) hexamers

Assembled icosahedron (h=1,k=2), T=7

Soccer ball (h=1,k=1), T=3

\[ \vec{a}_1 = (1, 0) \quad \vec{a}_2 = (1/2, \sqrt{3}/2) \]
Caspar-Klug classification of icosahedral capsids

Duality between hexagonal and triangular lattice

Pentamers correspond to vertices with 5 neighbors:

5-fold disclinations

Caspar-Klug classification of icosahedral capsids

Bacteriophage $\phi X$ 174

$T = 1$
$(h = 1, k = 0)$

Cowpea chlorotic mottle virus

$T = 3$
$(h = 1, k = 1)$

Simian virus SV40

$T = 7$
$(h = 1, k = 2)$

Capsids with Caspar-Klug numbers of type $(h,0)$ and $(h,h)$ have mirror symmetry, while other $(h,k)$ structures are chiral!

Why are viral capsids very often icosahedral?
Euler’s polyhedron formula

\[ V - E + F = 2 \]

V = number of vertices
E = number of edges
F = number of faces

tetrahedron
\[ V = 4 \]
\[ E = 6 \]
\[ F = 4 \]

cube
\[ V = 8 \]
\[ E = 12 \]
\[ F = 6 \]

octahedron
\[ V = 6 \]
\[ E = 12 \]
\[ F = 8 \]

icosahedron
\[ V = 12 \]
\[ E = 30 \]
\[ F = 20 \]
Euler’s polyhedron formula

\[ V - E + F = 2 \]

\( V \) = number of vertices
\( E \) = number of edges
\( F \) = number of faces

For arbitrary polyhedron constructed with triangles, the numbers of vertices, edges and faces are related:

Each face has 3 edges
Each edge is shared between 2 faces

The total number of vertices is given by:

\[ V = \sum_z N_z \]

The total number of edges is given by:

\[ E = \frac{1}{2} \sum_z z N_z \]

\[ 12 = \sum_z N_z (6 - z) \]
Euler’s polyhedron formula

\[ 12 = \sum_{z} N_z(6 - z) \]

- tetrahedron
  - \( N_3 = 4 \)
  - 3-fold disclinations

- octahedron
  - \( N_4 = 6 \)
  - 4-fold disclinations

- icosahedron
  - \( N_5 = 12 \)
  - 5-fold disclinations

- Caspar-Klug
  - \( h=3, k=1 \), \( T=13 \)
  - \( N_5 = 12 \)
  - \( N_6 = 10(T - 1) \)
  - \( N_6 = 120 \)

However, biological solutions of the Thomson problem were invented by viruses ~2-3 billion years ago…

Ordering on a sphere: 'geometric frustration' forces at least twelve 5-fold coordinated sites (= "disclinations") into the ground state…

Intermediate particle numbers are exhibited by the capsid shells of virus structures for 'magic numbers' of protein subunits indexed by pairs of integers \((P, Q)\).

\( \text{Simian virus } \text{SV40} \) \( (P, Q) = (1,2) \) \( (h=3, k=1), T=13 \)

z-fold disclination is associated with a topological charge

\[ q_z = \frac{\pi}{3} (6 - z) \]

total topological charge for closed convex polyhedra

\[ 4\pi = \sum_z N_z q_z \]

Note: dipoles of opposite charges (e.g. 5-fold and 7-fold disclinations) produce dislocations defects.
Topological charge vs Gaussian curvature

Triangulation of sphere

Gauss-Bonnet theorem

\[ 4\pi = \oint \frac{dA}{R_1 R_2} = \sum_z N_z q_z \]

Excess angle

Triangles on a sphere

\[ \alpha + \beta + \gamma > \pi \]

Excess angle over the edge of a curved surface

\[ \Delta \theta = \int \frac{dA}{R_1 R_2} = \sum_z N_z q_z \]
Buckling instability for disclinations

z-fold disclination is associated with a topological charge

\[ q_z = \frac{\pi}{3} (6 - z) \]

strain \[ \epsilon \sim q_z \]

stretching energy
\[ E_s \sim A \times Y \times \epsilon^2 \]
\[ E_s \sim Y R^2 q_z^2 \]
Y = 2D Young’s modulus

bending energy
(for the corresponding cone)
\[ E_b \sim \int dA \frac{\kappa}{(r/q_z)^2} \]
\[ E_b \sim \int rdr \frac{\kappa}{(r/q_z)^2} \]
\[ E_b \sim \kappa q_z^2 \ln(R/a) \]

buckling favorable for \[ R \gtrsim R_b \sim \sqrt{\kappa/Y} \]
Buckling instability for disclinations

\[ E_s \sim Y R^2 q_z^2 \]

\[ E_b \sim \kappa q_z^2 \ln(R/a) \]

\[ R_b \sim \sqrt{\kappa/Y} \]

H.S. Seung and D.R. Nelson,
PRA 38, 1005 (1988)
Buckling instability for spherical shells with 12 5-fold disclinations.

\[ \frac{\langle \Delta R^2 \rangle}{R^2} = Y \frac{R^2}{\kappa} \]

\( \gamma = Y \frac{R^2}{\kappa} \)

- Simian virus SV40, \( R \approx 25 \text{nm} \)
- Paramecium Bursana Chlorella Virus, \( R \approx 93 \text{nm} \)

Note: viral capsids may have non-zero spontaneous curvature!

J. Lidmar et al., PRE 68, 051910 (2003)
Icosahedral viral capsids

Topology requires certain number of disclinations

\[ 12 = \sum_{z} N_z (6 - z) \]

5-fold disclinations have lower energy than 4-fold and 3-fold disclinations. 7-fold and 8-fold disclinations would have to be compensated by additional 5-fold disclinations.

12 5-fold disclinations want to be as far away as possible, which produces structures with icosahedral symmetry.
Bacteriophage T4 infecting bacteria

Before attachment to bacteria the virus tail is in the extended state.

After attachment to bacteria the virus tail contracts and the hard inner core tube pierces through bacteria cell wall. Then viral DNA enters the cell through the tube.

50nm
Contraction of Bacteriophage T4 tail

Contraction of the virus tail is achieved by movement of dislocations (5-fold + 7-fold disclination) through the tail.

movement of dislocations modifies the crystal orientation on tail sheet