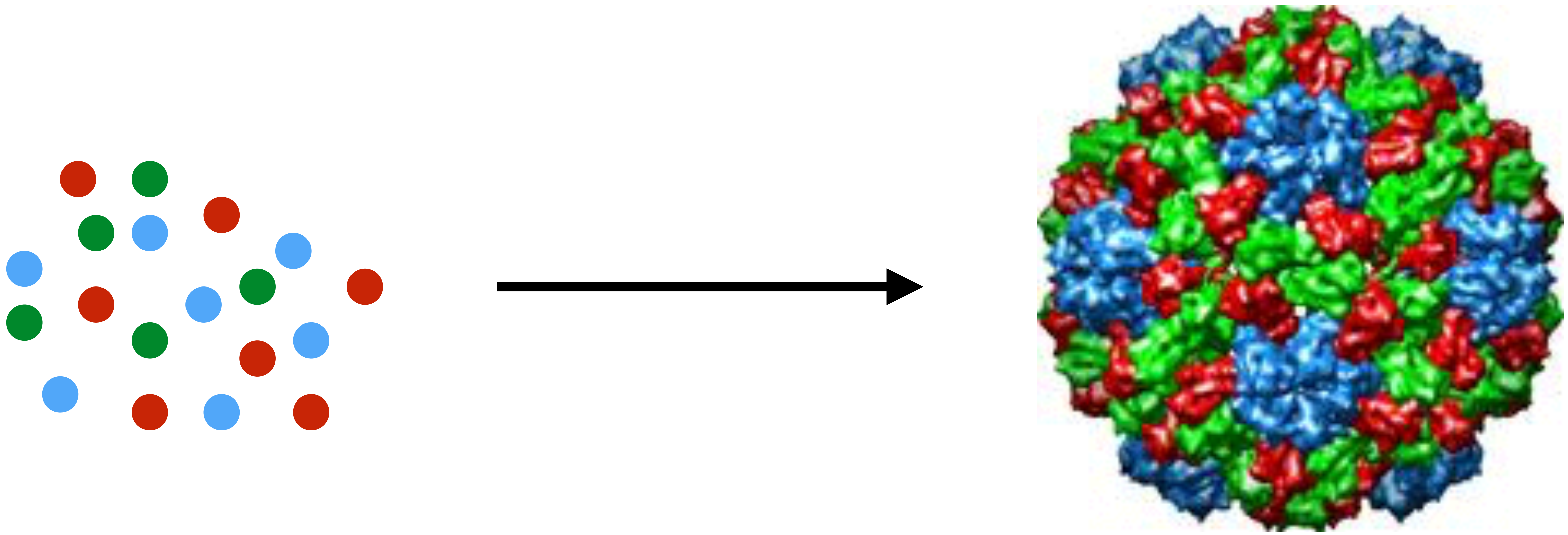
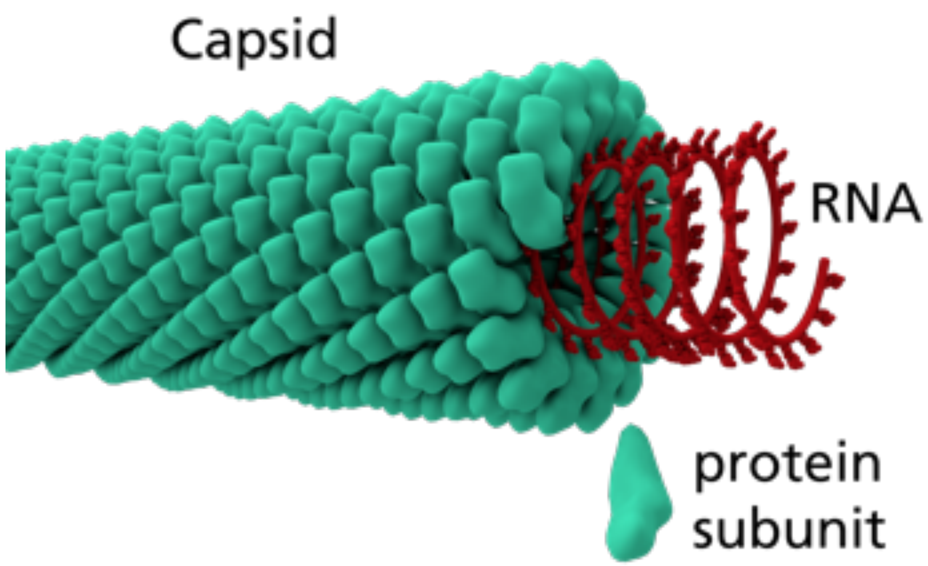
## MAE 545: Lecture 22 (12/10)

# Viral capsids and self assembly



# Viral capsids

## helical symmetry

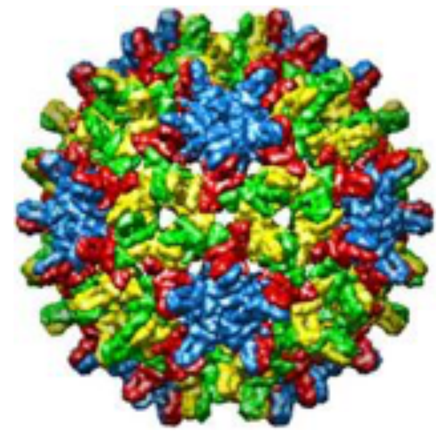



capsid proteins are wrapped around the viral RNA

(e.g. Tobacco Mosaic Virus)

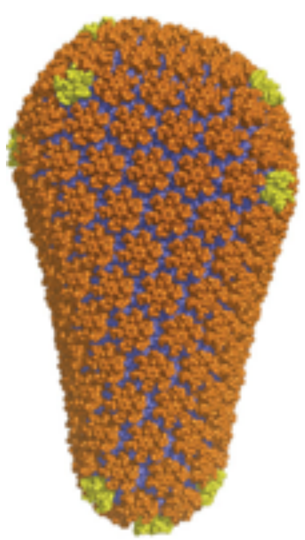
Note: many viruses also have envelope (lipid bilayer) around the capsid

## icosahedral symmetry



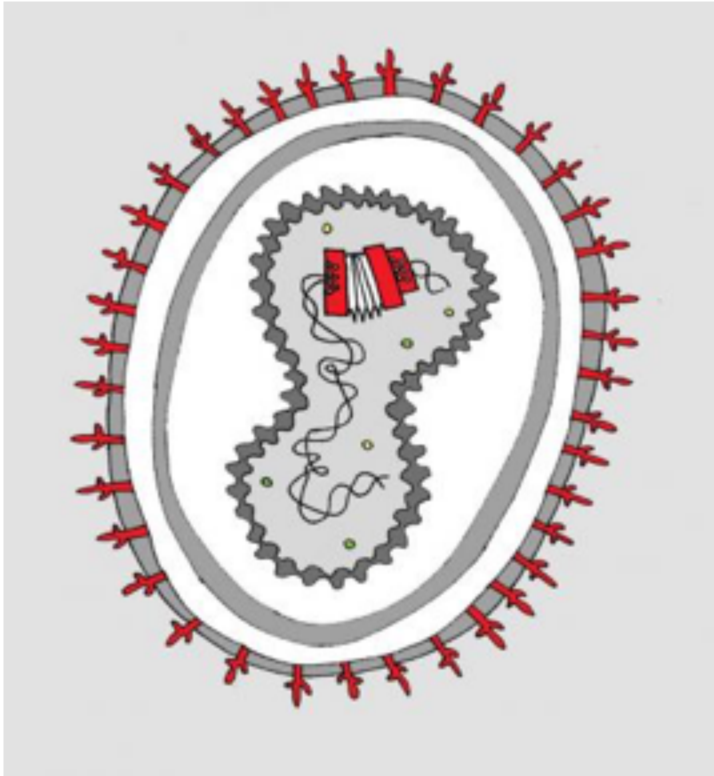
Hepatitis B virus

## conical shaped (spherical caps usually still icosahedral)



HIV

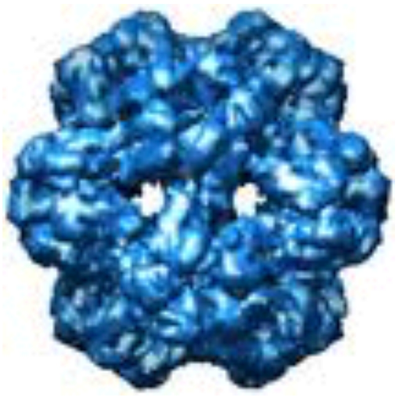
## complex symmetry



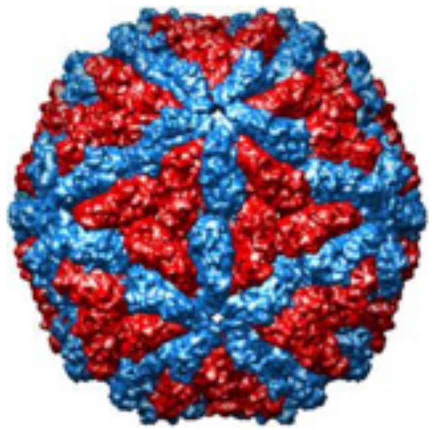
Poxvirus

# Icosahedral capsids

Brome mosaic virus

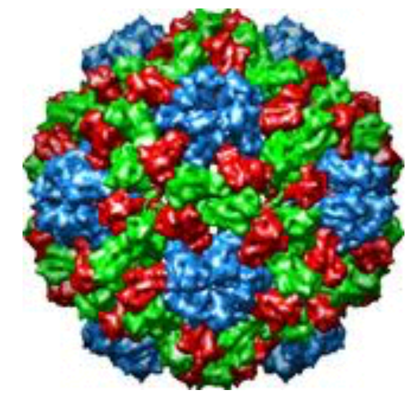


L-A virus

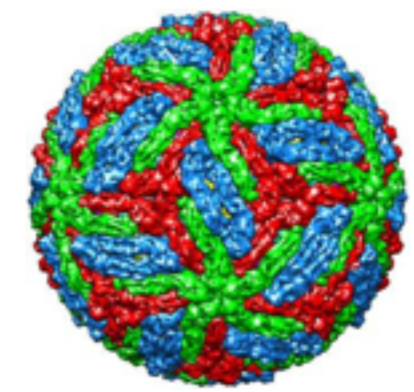


Bacteriophage $\phi$X 174

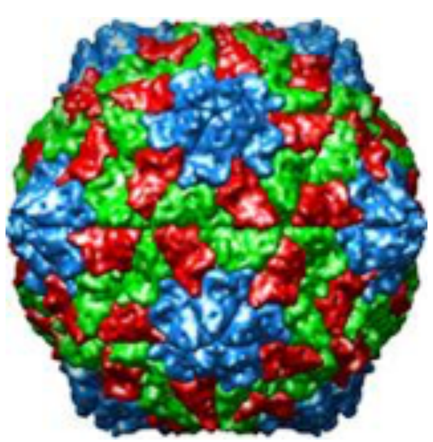
Cowpea Chlorotic Mottle virus



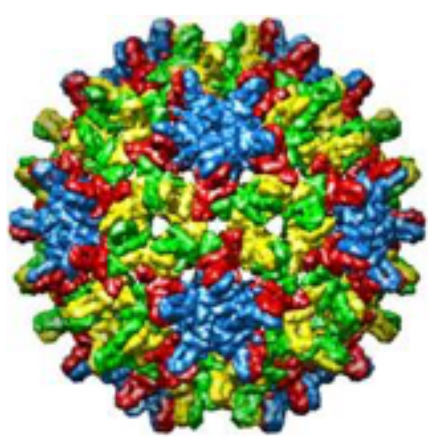
Dengue virus



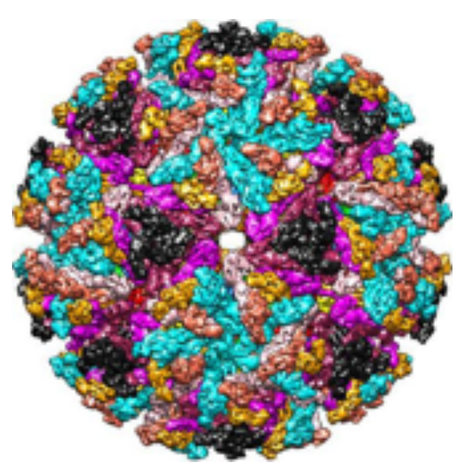
Tobacco Necrosis virus



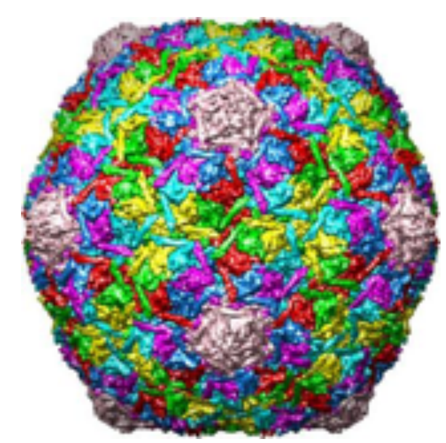
Human Hepatitis B Virus



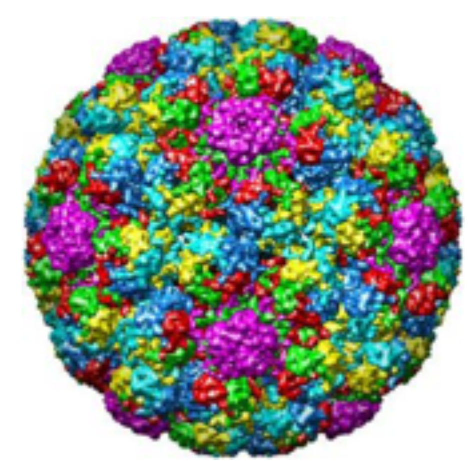
Sindbis virus



Bacteriophage HK97



Simian virus

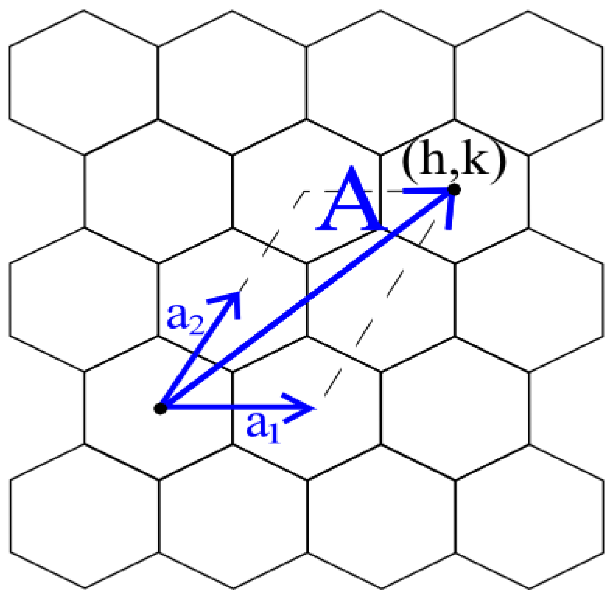


**Colors correspond to different proteins.**

# Caspar-Klug classification of icosahedral capsids

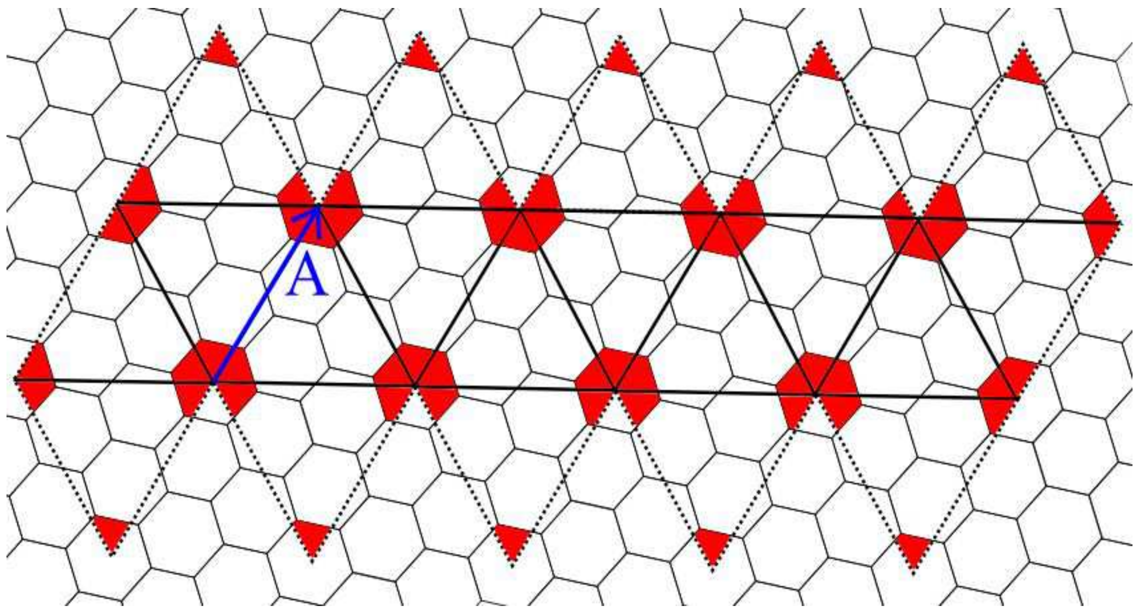
**Generating vector**

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

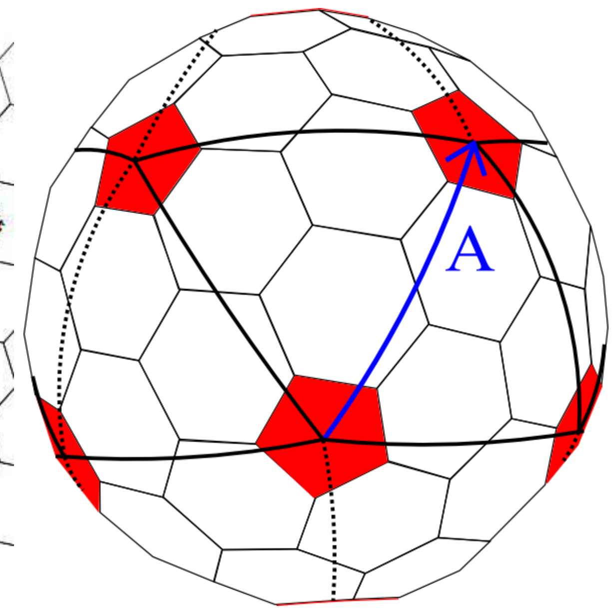



$\vec{a}_1 = (1,0) \qquad \vec{a}_2 = (1/2, \sqrt{3}/2)$

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




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



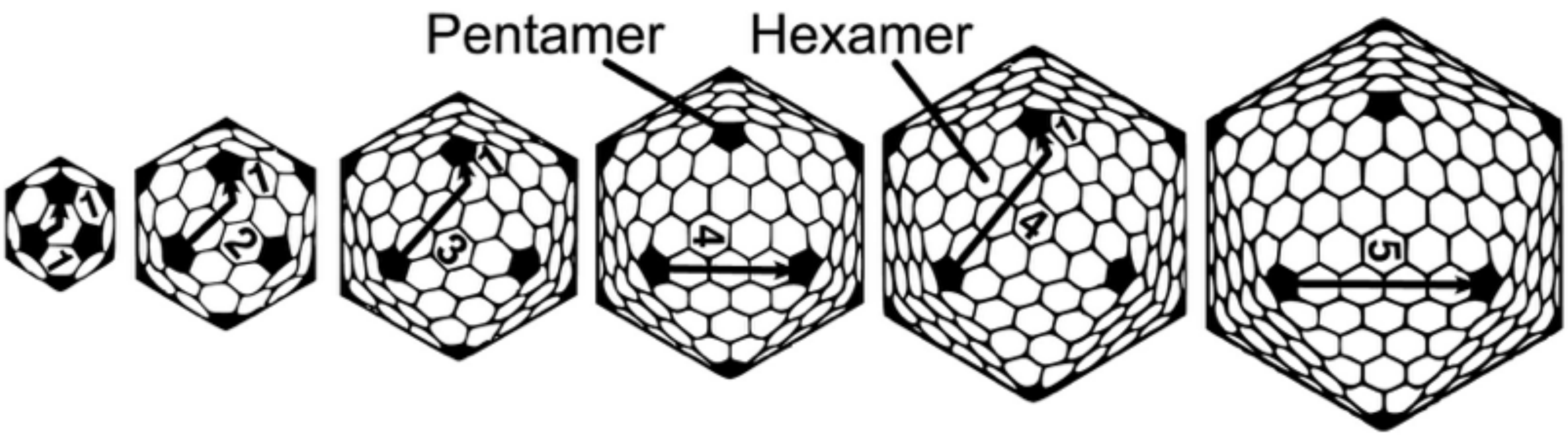

**T number:** $$T = \vec{A}^2 = h^2 + k^2 + hk$$

**12 pentamers (vertices of icosahedron)**

**10 (T-1) hexamers**

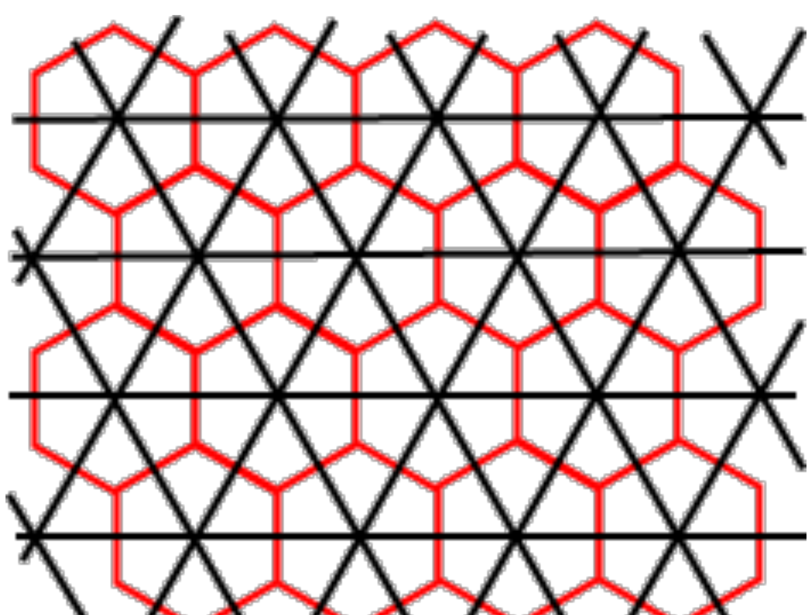
**Soccer ball (h=1,k=1), T=3**

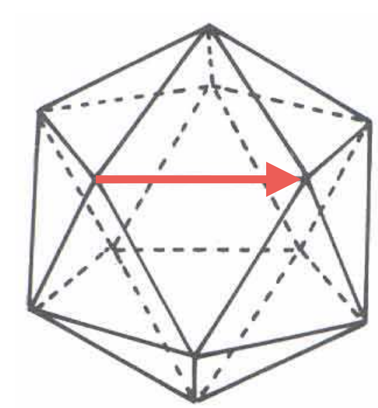
# Caspar-Klug classification of icosahedral capsids

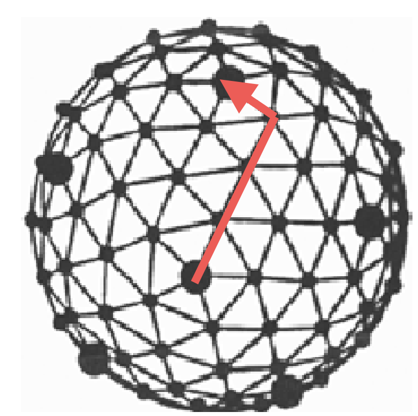



| | | | | | | |
|---|---|---|---|---|---|---|
| $T=$ | 3 | 7 | 13 | 16 | 21 | 25 |
| $(h,k)=$ | (1,1) | (2,1) | (3,1) | (4,0) | (4,1) | (5,0) |

## Duality between hexagonal and triangular lattice







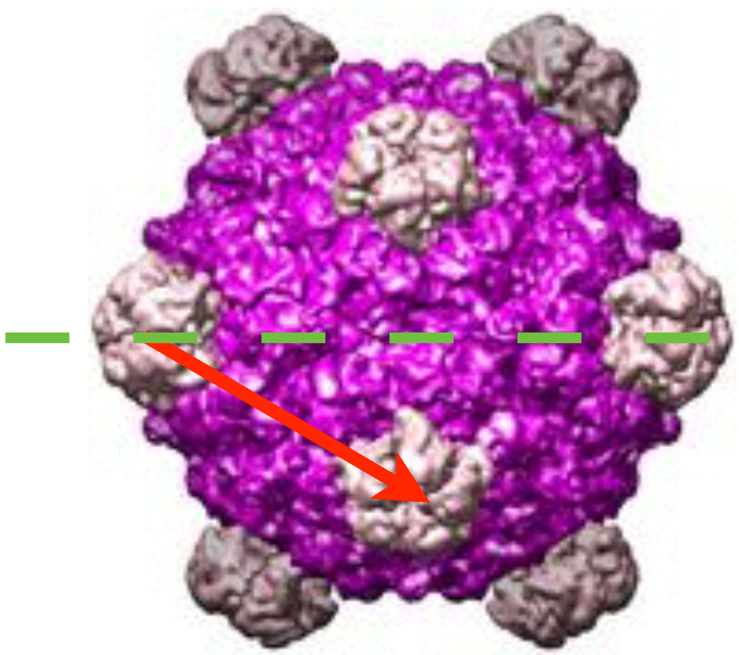
| | | |
|---|---|---|
| $T=$ | $1$ | $13$ |
| $(h,k)=$ | $(1,0)$ | $(3,1)$ |

**Pentamers correspond to vertices with 5 neighbors:**

**5-fold disclinations**

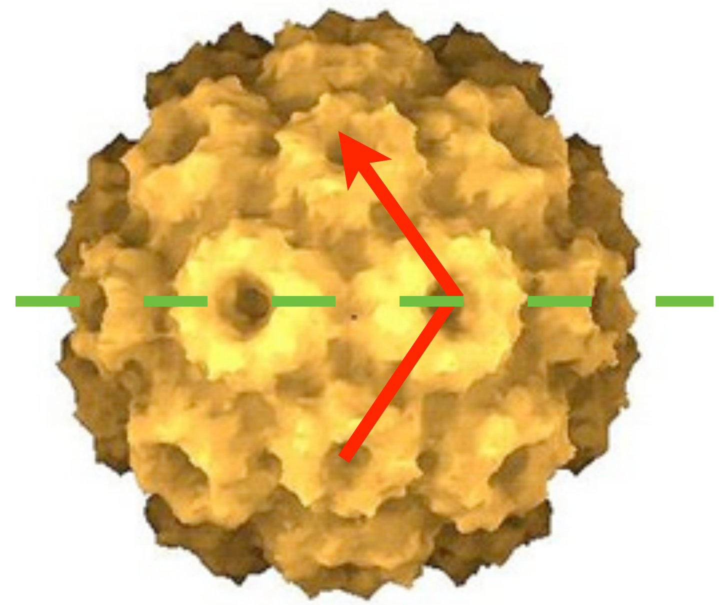
# Caspar-Klug classification of icosahedral capsids

**Bacteriophage $\phi$X 174**



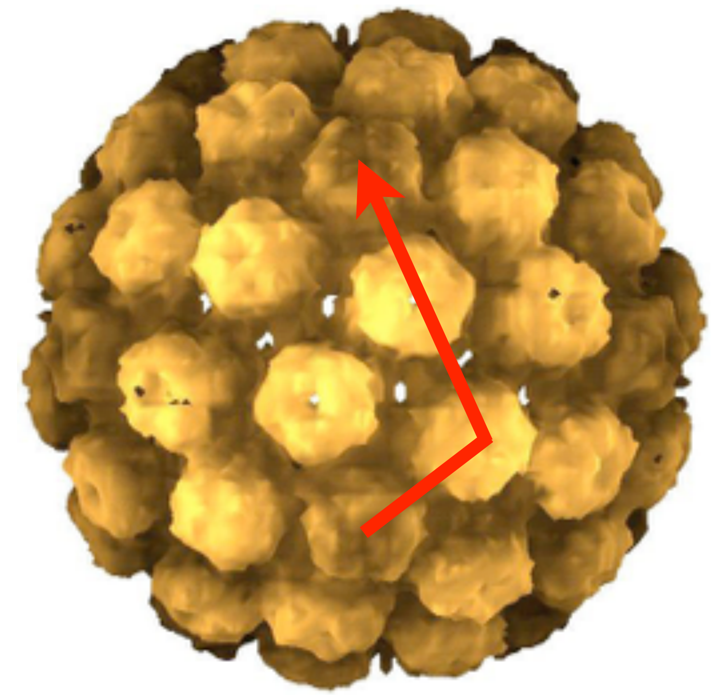
$$T = 1$$
$$(h = 1, k = 0)$$

**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**

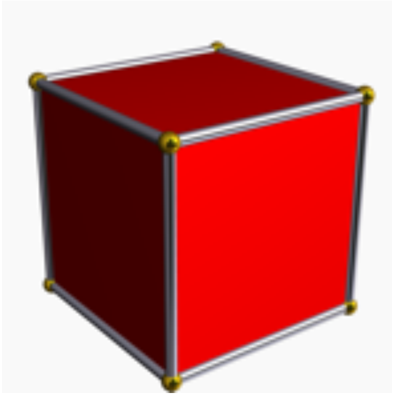
## tetrahedron

$$V = 4$$
$$E = 6$$
$$F = 4$$

## octahedron

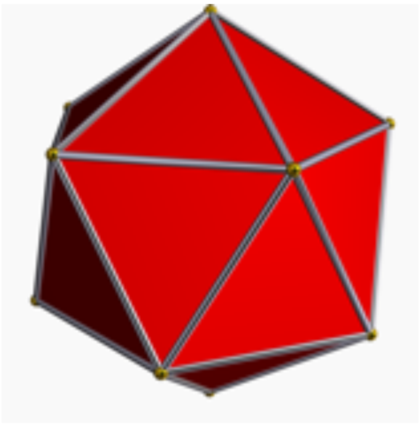
$$V = 6$$
$$E = 12$$
$$F = 8$$

## cube



$$V = 8$$
$$E = 12$$
$$F = 6$$

## icosahedron



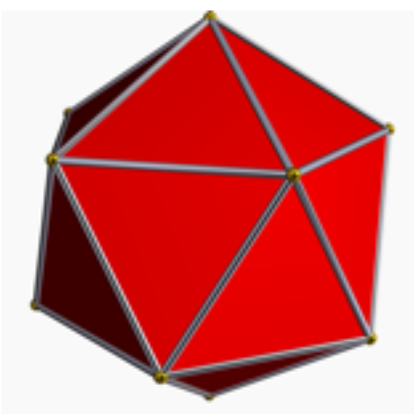
$$V = 12$$
$$E = 30$$
$$F = 20$$

# 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:**



$$E = \frac{3F}{2}$$

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

$$N_z$$

number of vertices with *z* neighbors

$$V = \sum_z N_z$$

total number of vertices

$$E = \frac{1}{2} \sum_z z N_z$$

total number of edges

$$V - E + F = 2 \quad \longrightarrow \quad 12 = \sum_z N_z (6 - z)$$

# Euler's polyhedron formula

$$12 = \sum_z N_z(6 - z)$$

**tetrahedron**

$N_3 = 4$

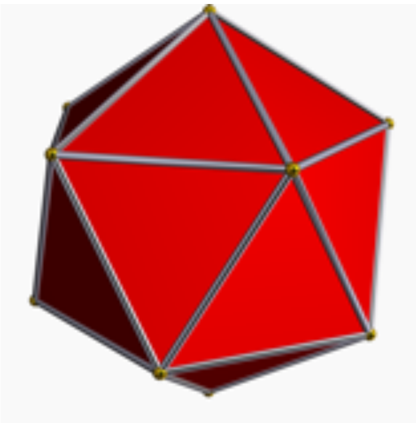
**3-fold disclinations**

**octahedron**

$N_4 = 6$

**4-fold disclinations**

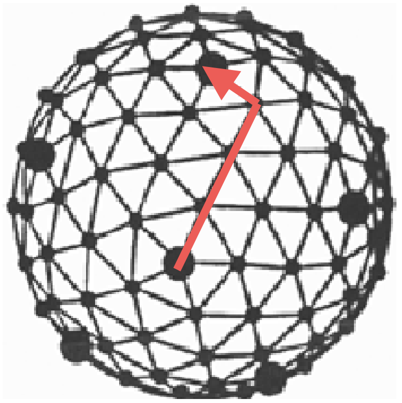
**icosahedron**



$N_5 = 12$

**5-fold disclinations**

**Caspar-Klug (h=3, k=1), T=13**



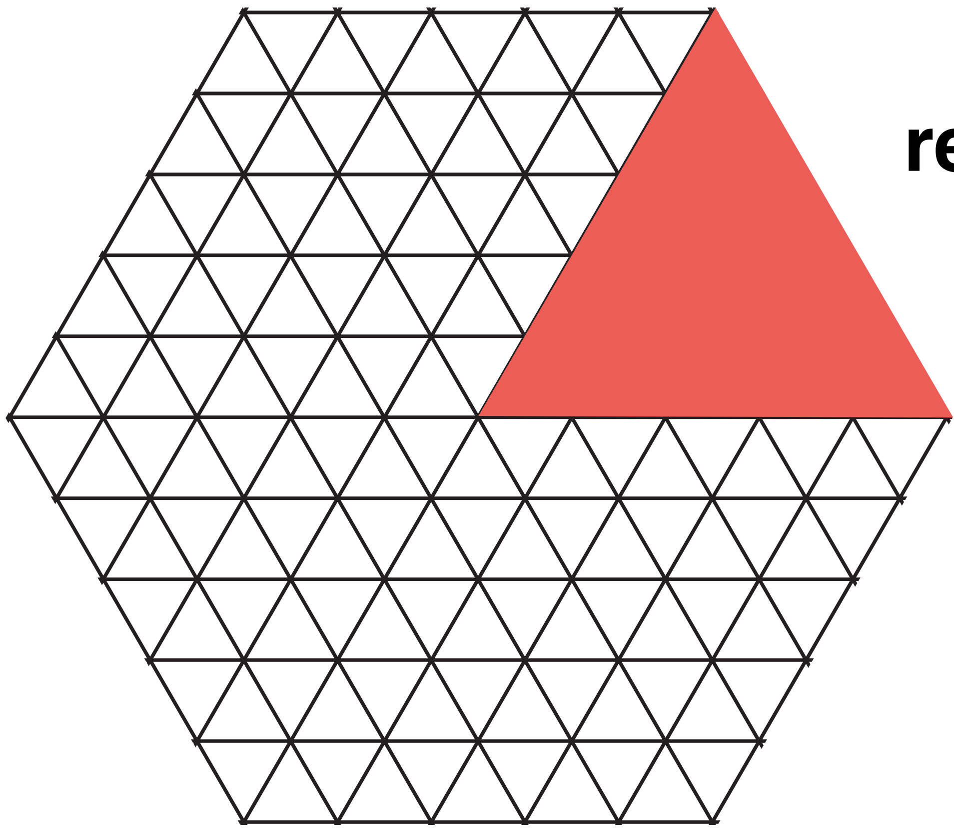
$N_5 = 12$

$N_6 = 10(T - 1)$

$N_6 = 120$

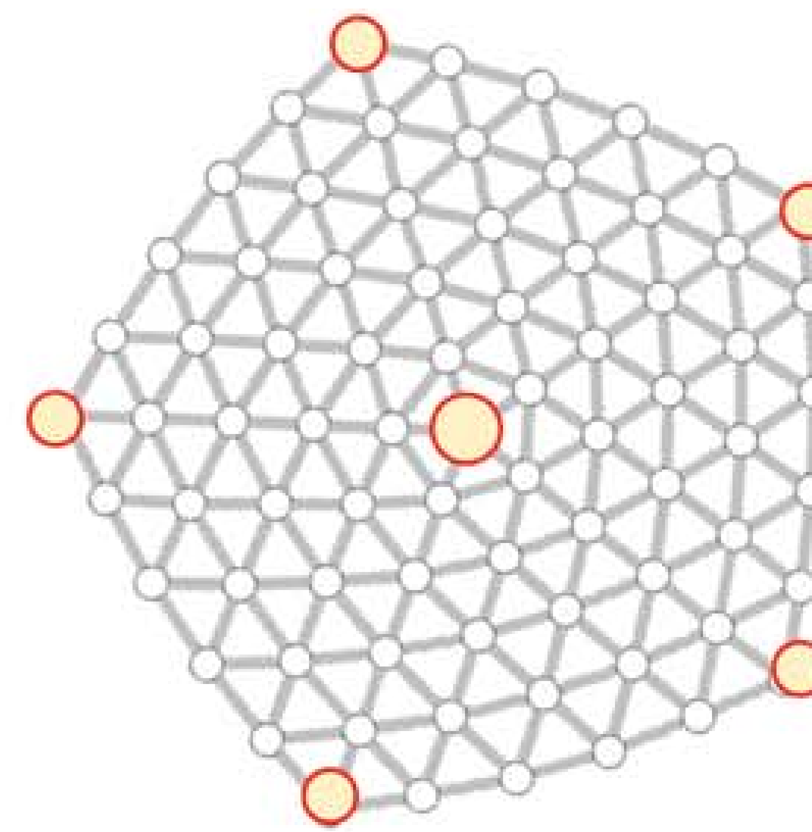
**5-fold disclinations**

# Topological charge of disclinations



remove a wedge
of angle $\pi/3$

5-fold disclination



**z-fold disclination is associated with a topological charge**

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

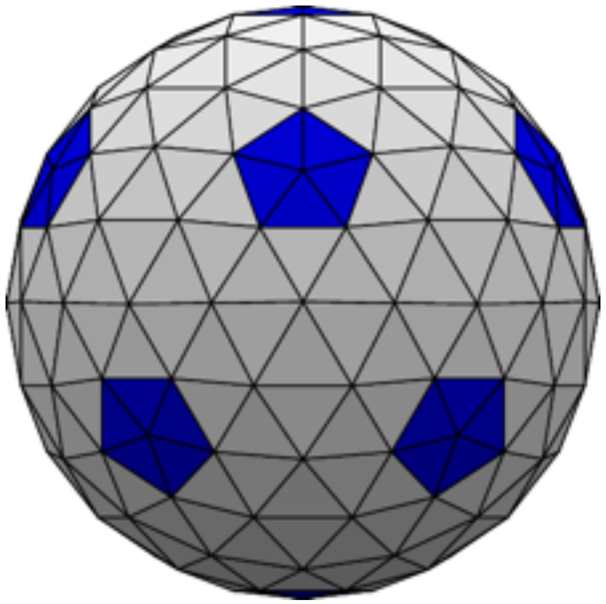
**total topological charge for closed convex polyhedra**

$$4\pi = \sum_z N_z q_z$$

**Note: dipoles of opposite charges (e.g. 5-fold and 7-fold disclinations) produce dislocations defects.**

# Topological charge vs Gaussian curvature

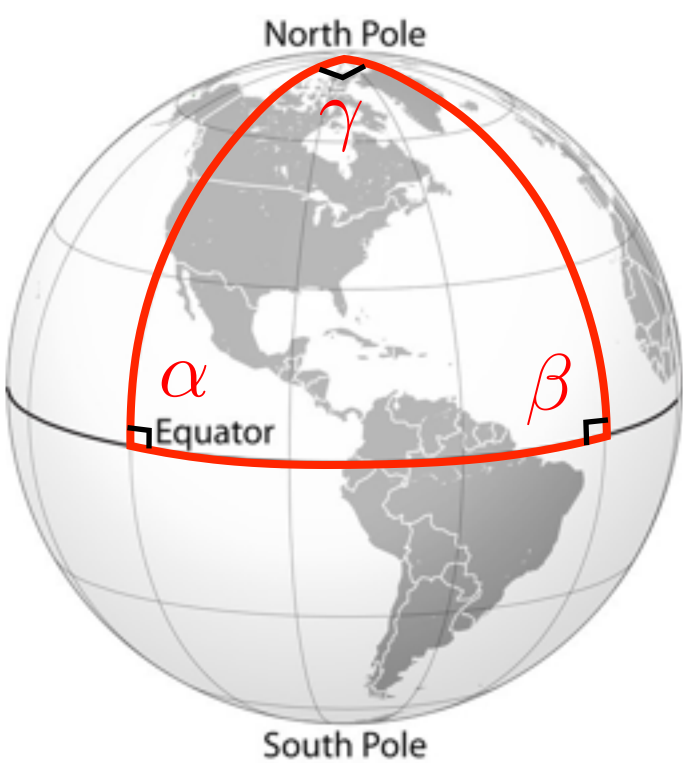
**Triangulation of sphere**



**Gauss-Bonnett theorem**

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

## Excess angle




**Triangles on a sphere**

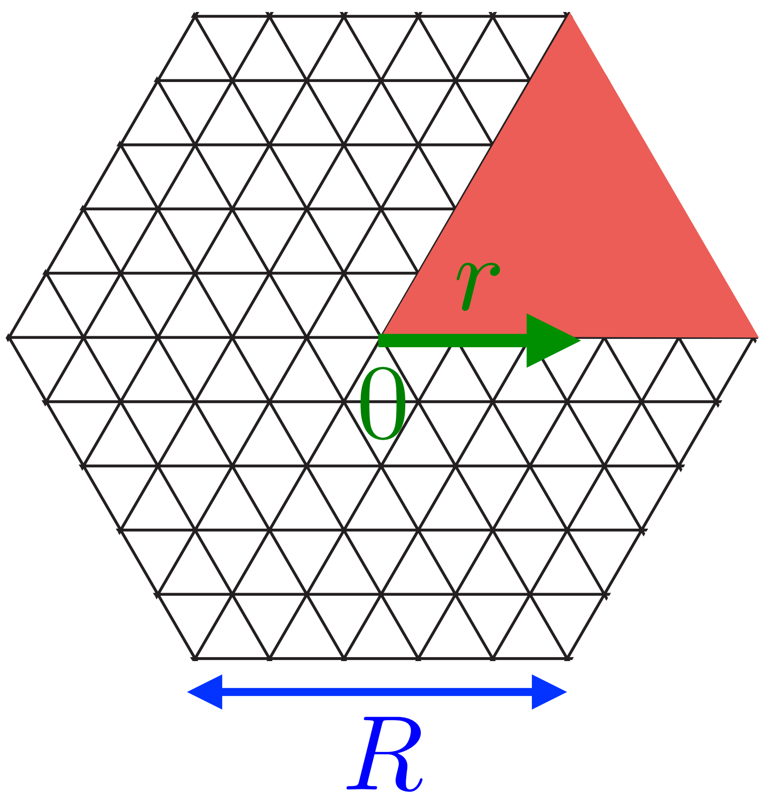
$$\alpha + \beta + \gamma > \pi$$

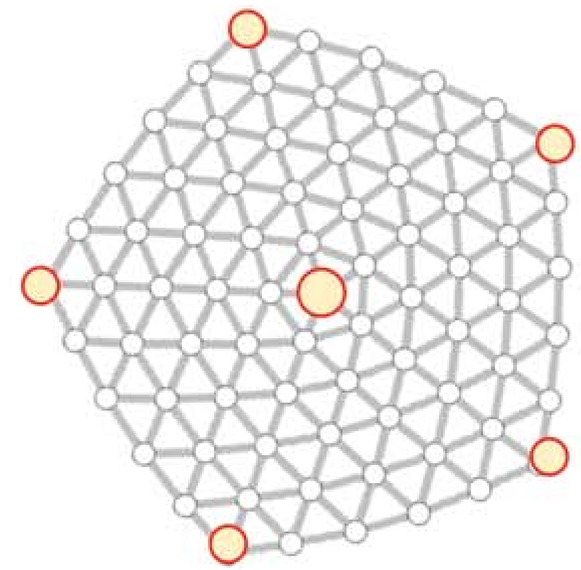
**Excess angle over the edge of a curved surface**

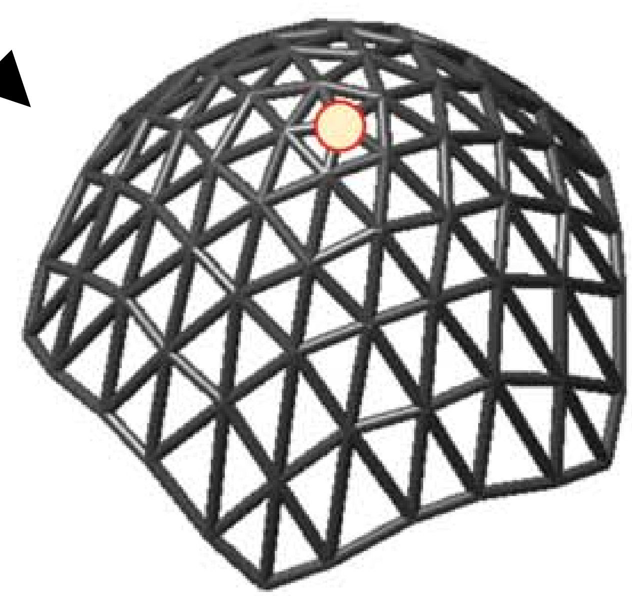
$$\Delta\theta = \int \frac{dA}{R_1 R_2} = \sum_z N_z q_z$$

# Buckling instability for disclinations

**remove a wedge of angle $\pi/3$**





**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)**

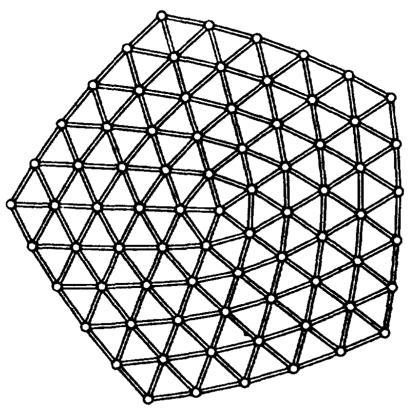
$$E_b \sim \int dA \frac{\kappa}{(r/q_z)^2}$$

$$E_b \sim \int r dr \frac{\kappa}{(r/q_z)^2}$$

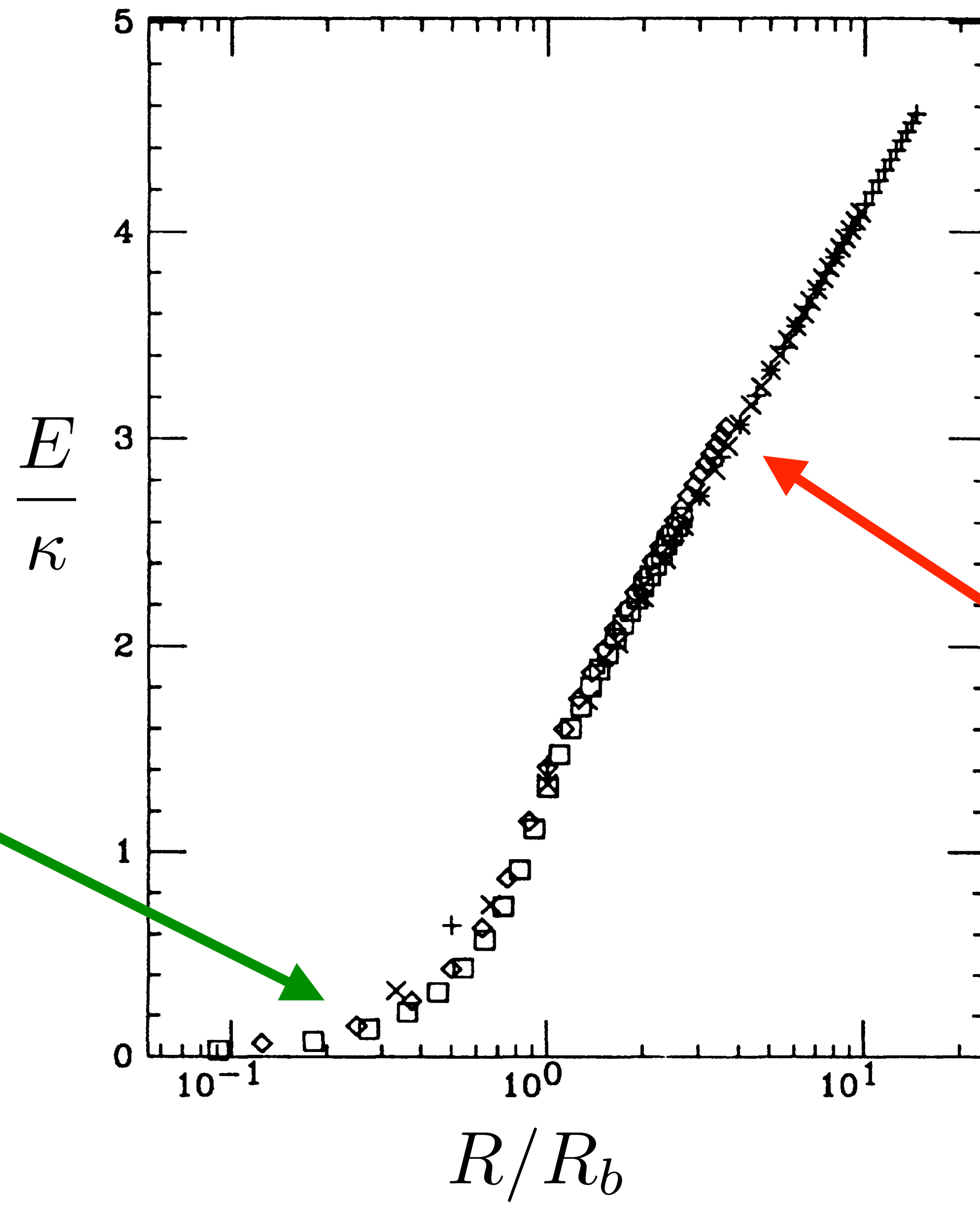
$$E_b \sim \kappa q_z^2 \ln(R/a)$$

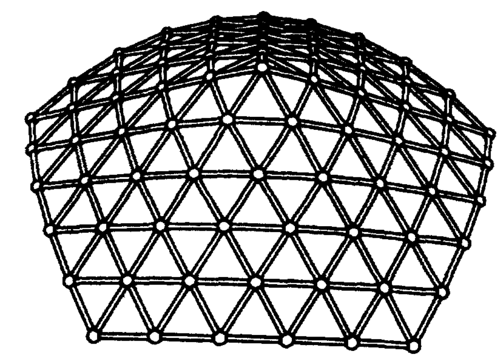
**buckling favorable for** $R \gtrsim R_b \sim \sqrt{\kappa/Y}$

# Buckling instability for disclinations



$$E_s \sim Y R^2 q_z^2$$



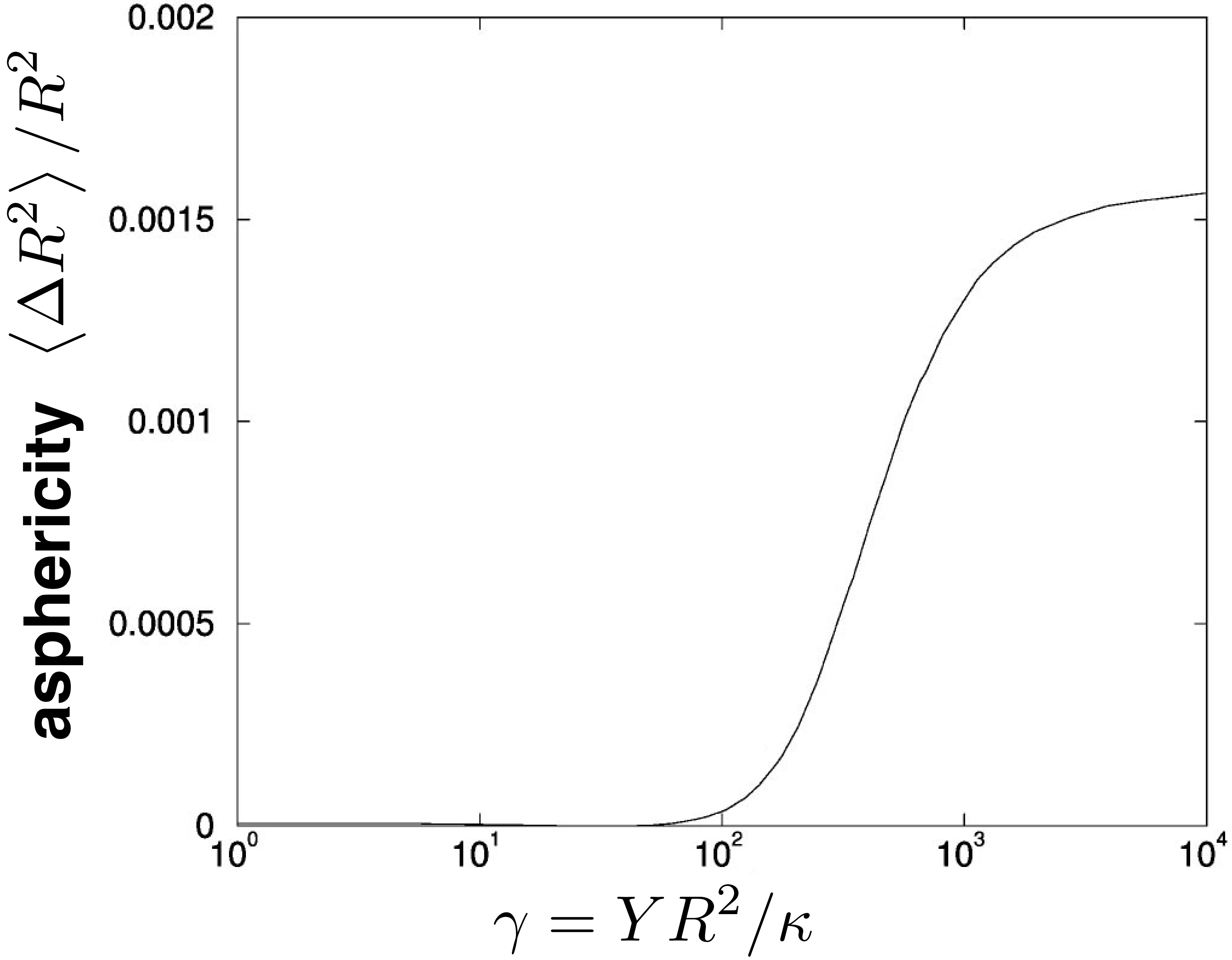



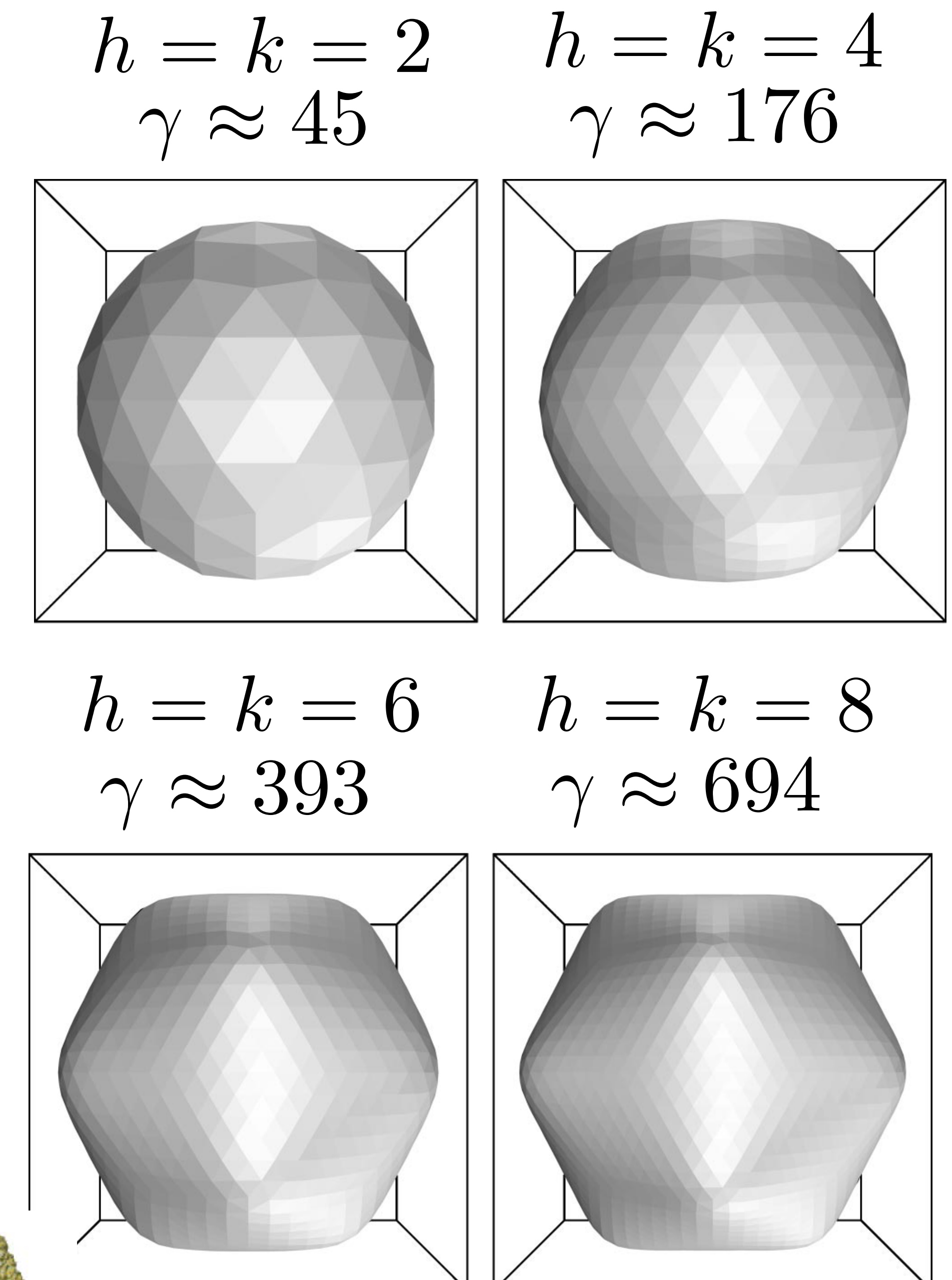
$$E_b \sim \kappa q_z^2 \ln(R/a)$$

$$R_b \sim \sqrt{\kappa/Y}$$

H.S. Seung and D.R. Nelson,
PRA 38, 1005 (1988)

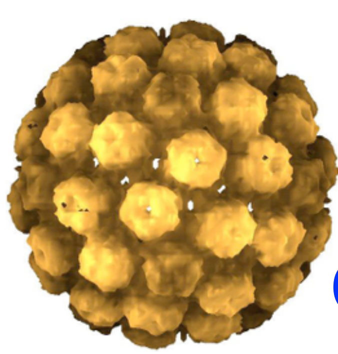
# Buckling instability for spherical shells with 12 5-fold disclinations



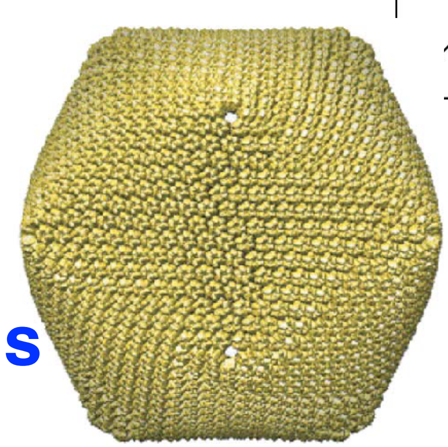




**Simian virus SV40**

$R \approx 25\text{nm}$



**Paramecium Bursana Chlorella Virus**



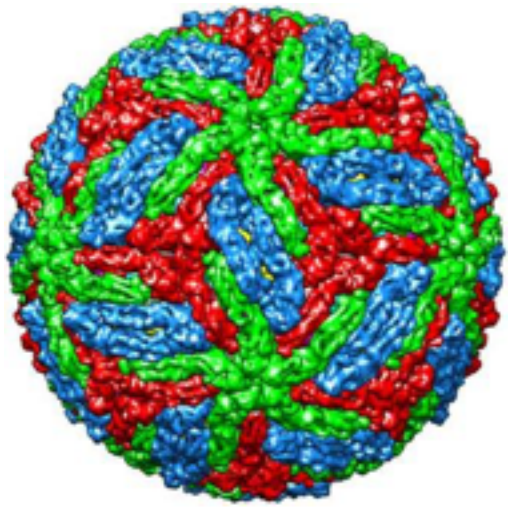
$R \approx 93\text{nm}$

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



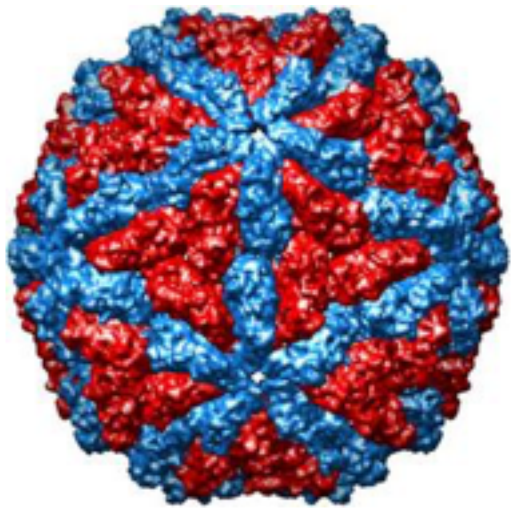
J. Lidmar et al., PRE 68, 051910 (2003)

# Icosahedral viral capsids

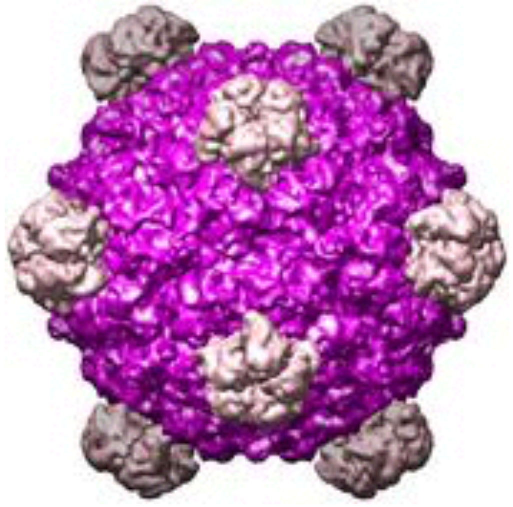


**Topology requires certain number of disclinations**

$$12 = \sum_z N_z(6 - z)$$

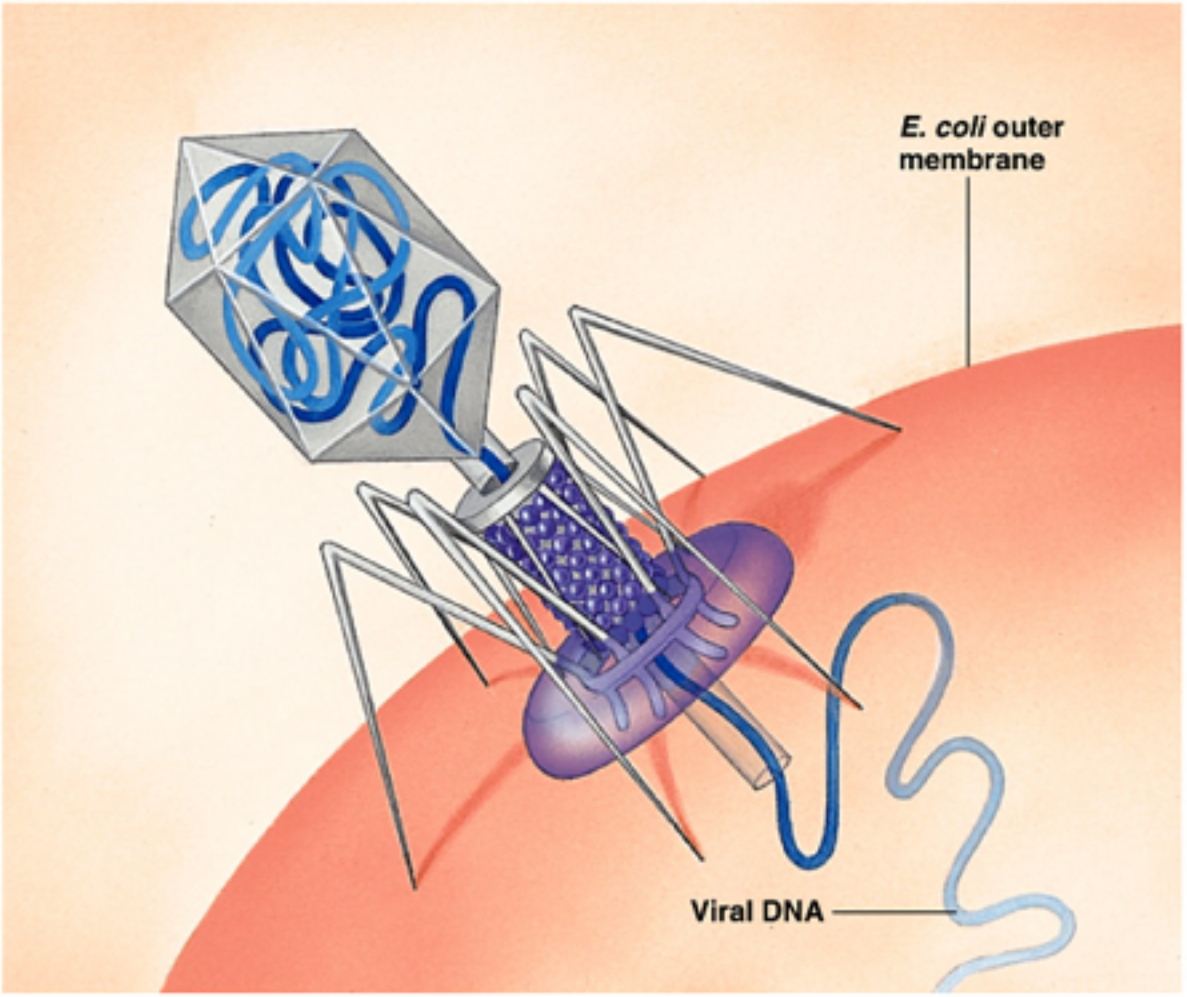


**5-fold disclinations have lower energy then 4-fold and 3-fold disclinations. 7-fold and 8-fold disclinations would have to be compensated by additional 5-fold disclinations.**

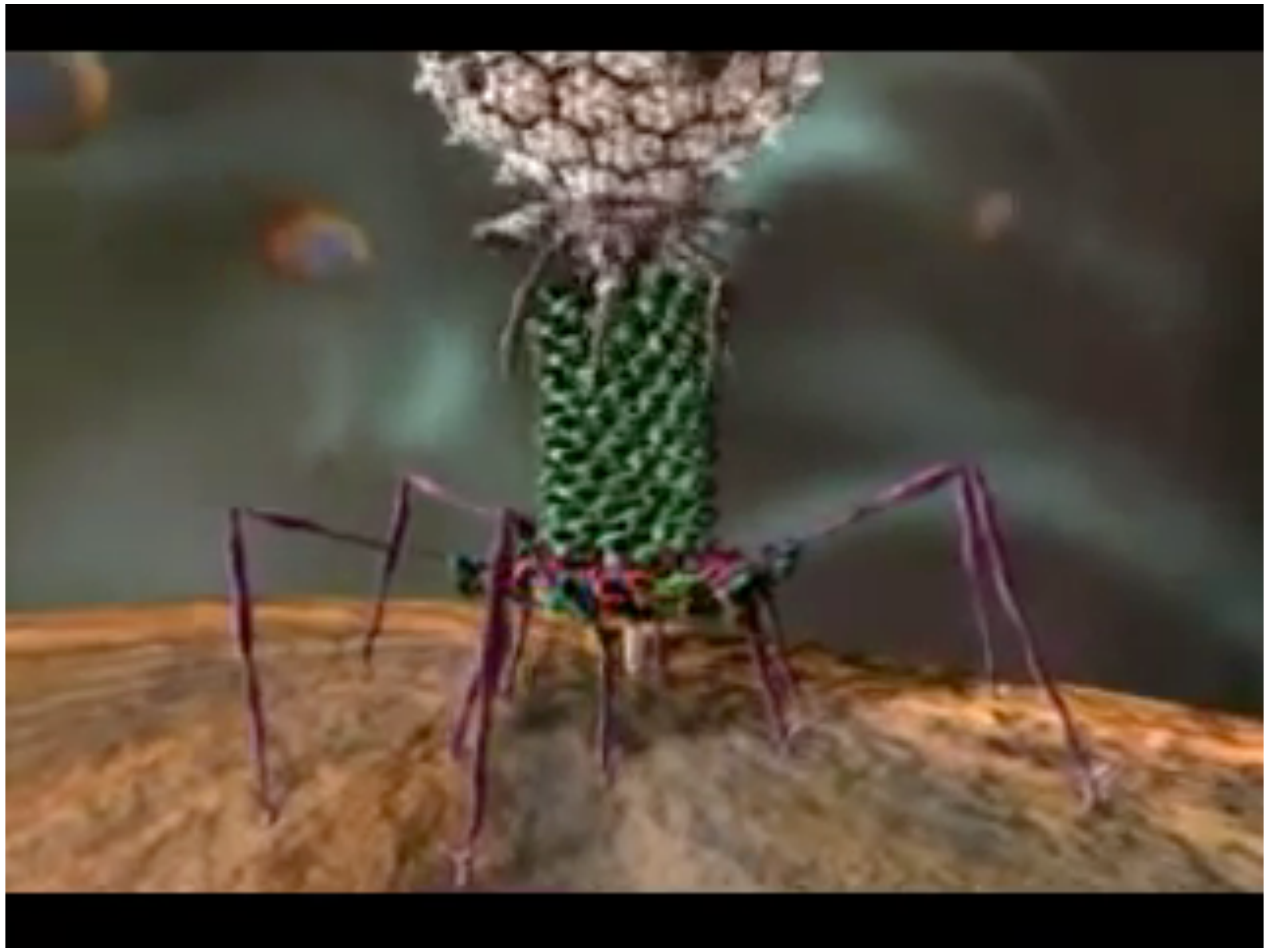


**12 5-fold disclinations want to be as far away as possible, which produces structures with icosahedral symmetry.**

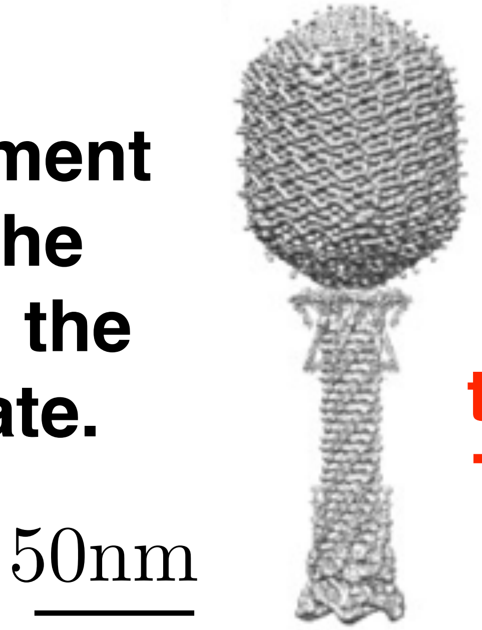
# Bacteriophage T4 infecting bacteria



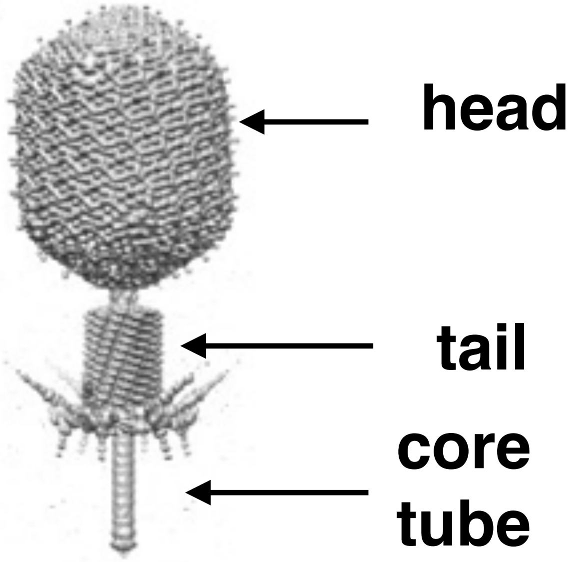


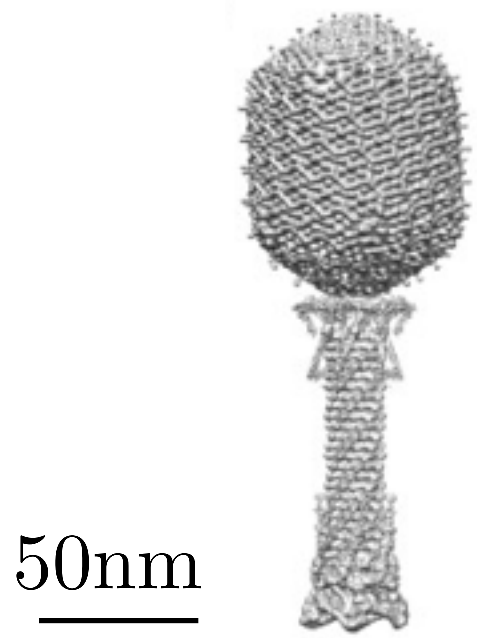
**Before attachment to bacteria the virus tail is in the extended state.**



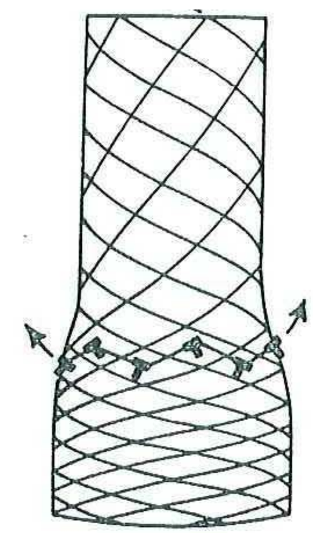

**After attachment to bacteria the virus tail contracts and the hard inner core tube pierces through bacteria cell wall. Then viral DNA enters the cell through the tube.**

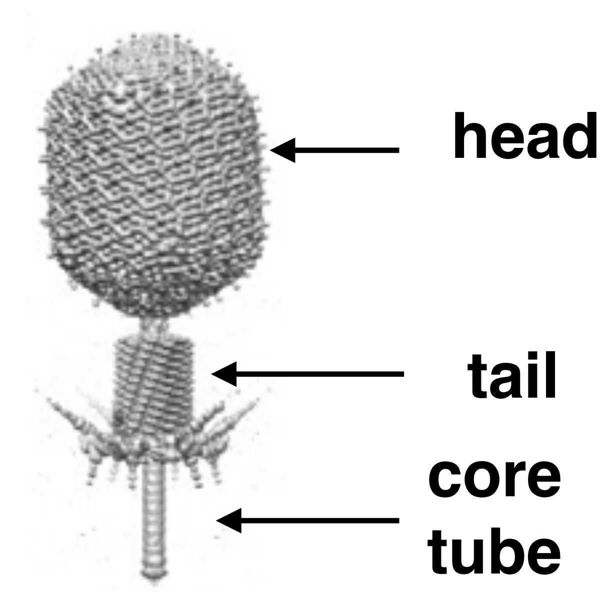


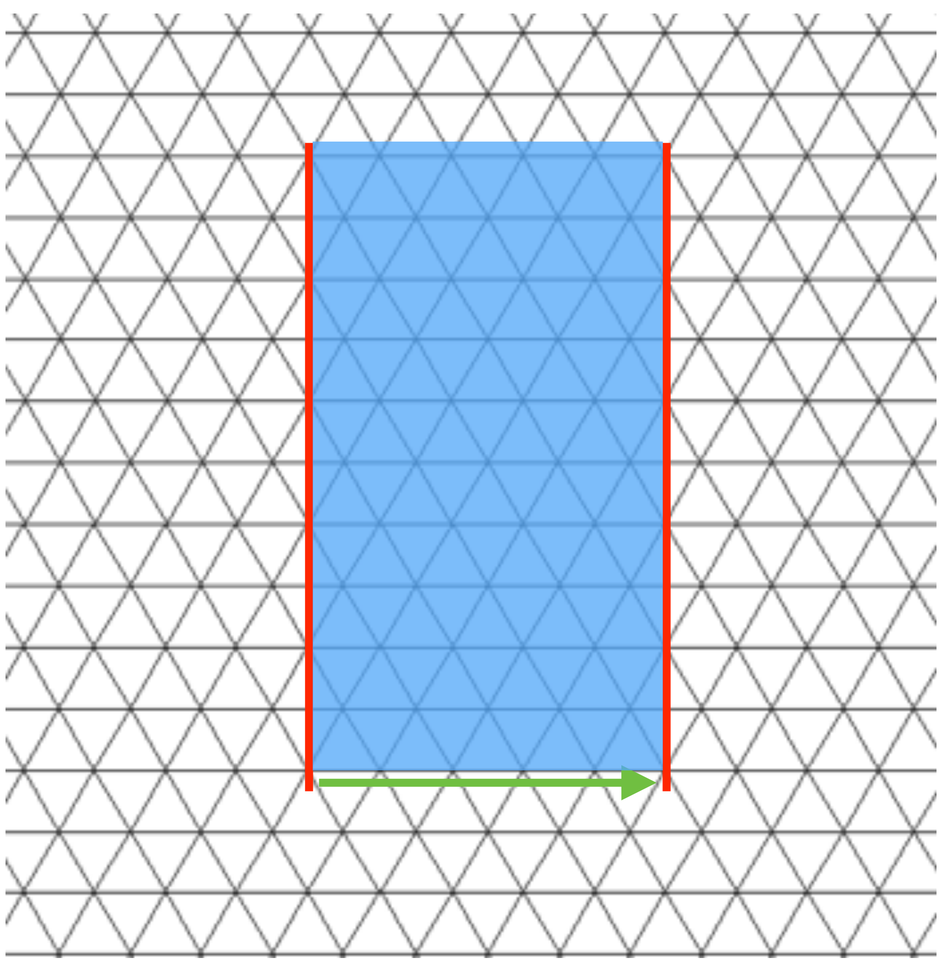
# Contraction of Bacteriophage T4 tail




**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**