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3.22 Mechanical Properties of Materials
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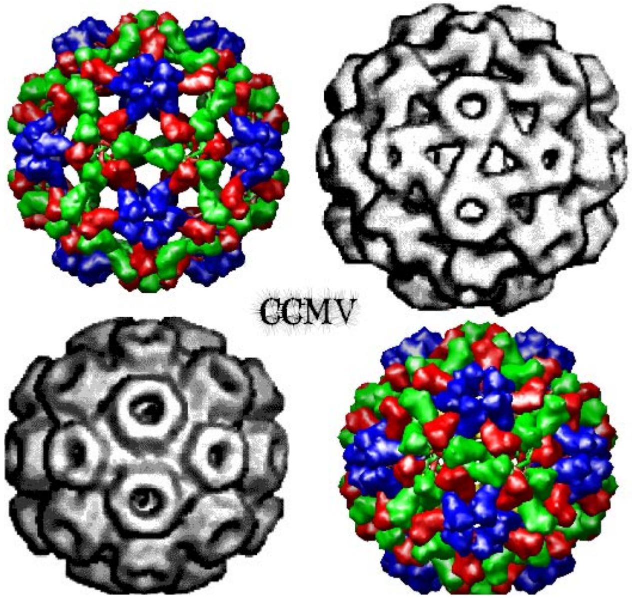
Mechanical Behavior of a Virus



cowpea chlorotic mottle virus

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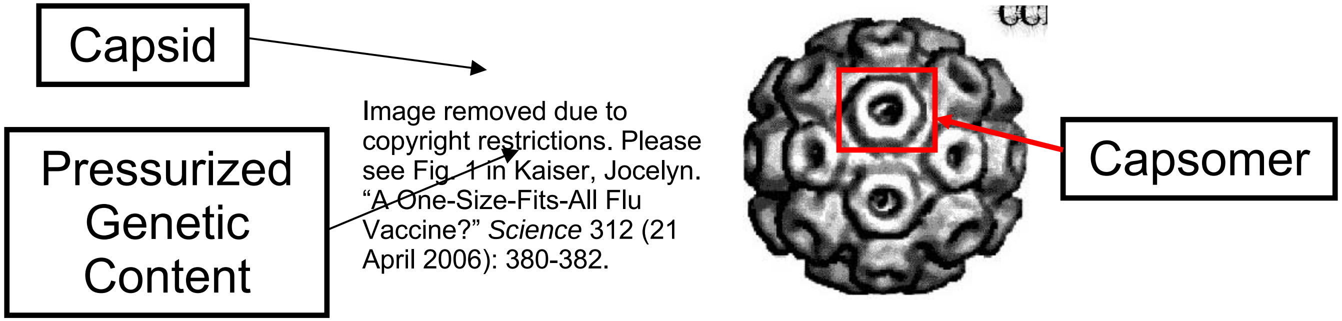
Big Picture

- **Phenonmenon: Failure of viral capsids**
  - Viral capsids = proteinaceous outer shell of viruses that enclose highly-packed genetic material under high pressure
  - Capsomers = subunits that make up the capsid



Capsid

Pressurized Genetic Content

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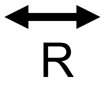
Capsomer

- **Material Class:** Proteinaceous biological materials
- **Motivation:**
  - Understanding viral release of genetic materials
  - Gene therapy
  - Biomimetic nanocontainers for drug delivery
  - Antiviral Vaccines

Microscopic mechanism

- **Lennard-Jones Potential Model**
  - Explains the equilibrium structure of viral capsids.
  - Force Balance: R<R(eq.): Repulsive force = Compressive stress
    R>R(eq.): Attractive force = Tensile stress

a) b)



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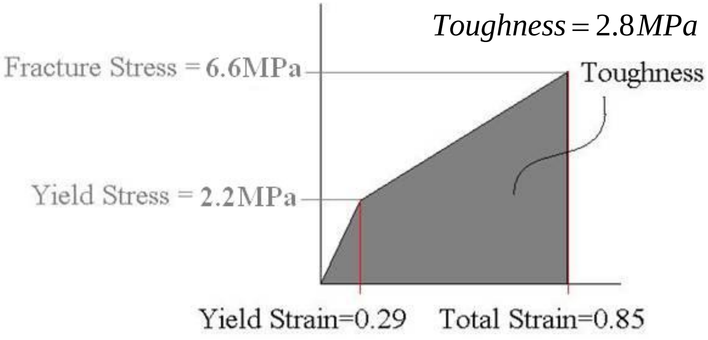
Please see Fig. 1a and 5 in [1], and
http://commons.wikimedia.org/wiki/File:Argon_dimer_potential_and_Lennard-Jones.png

- Asymmetric L-J potential explains the stress states seen in Figure b).
  - Compressive stress at R<R(eq.) decreases faster with R than the tensile stress does at R>R(eq.)

- **Mechanical probing of virus capsids**
  - Atomic force microscopy (AFM) used to strain the capsid until yielding and then fracture occur. Toughness and yield stress can be calculated.

$$\sigma_y = \frac{F_{yield}}{Area} = \frac{2.8nN}{1252.2nm^2} = 2.2MPa$$



[1] Zandi, R., and D. Reguera. “Mechanical properties of viral capsids.” *Physical Review E* 72 (2005): 021917.

Prediction & Optimization

- **Predictions**:
  - Equilibrium capsomer spacing → ***Equilibrium capsid radius, R***
  - Asymmetric LJ potential → Easier (smaller required σ) to stretch than compress by a given ΔR
    - ***Capsids more easily fail by bursting/rupture than by compression!***
  - LJ potential between capsomers →
    - Max tolerable force (+ accompanying radius) found from potential's flex point
      - ***5-10% radius expansion before bursting***
  - With increasing thermal fluctuations at increasing T →
    - ***Capsids fail before flex point radius and stress at higher T***

- **Optimization**:
  - To enhance bursting (genetic material delivery):
    - Increase T
    - Adjust pH & salt concentrations of ambient environment to increase differential osmotic pressure
      - i.e. decrease ambient pressure

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Upon bursting, small crack develops which propagates catastrophically until it rips across capsid surface

As in intergranular fracture, the crack propagates most easily at the interface between adjacent capsomers

[1] Zandi, R., and D. Reguera. "Mechanical properties of viral capsids." *Physical Review E* 72 (2005): 021917.