Outline

• Stretching
  Stress
  Strain
  \(\text{Stress-Strain curve}\)

• Mechanical Properties
  Young’s modulus
  Strength
  Ultimate strain
  Toughness modulus

• Size effects on energy dissipated
• Linear Elastic Fracture Mechanics (LEFM)
  Stress-intensity factor
  Energy release rate
  Fracture toughness
  Size-effect on fracture strength

• Quantized Fracture Mechanics (QFM)
  Strength of graphene (and related materials)

• Bending
  Flexibility
  Bending stiffness
  Elastic line equation
  Elastic plate equation
Exercises by me

1. Apply QFM for deriving the strength of realistic thus defective graphene (and related 2D materials);
2. Apply LEFM for deriving the peeling force of graphene (and related 2D materials).

Exercises by you

1. Apply LEFM for measuring the fracture toughness of a sheet of paper;
2. Apply the Bending theory for calculating the maximal curvature before fracture.
Stretches

Fiber under tension

Stress:  \( \sigma = \frac{F}{A} \)

Strain:  \( \varepsilon = \frac{\Delta l}{l} \)
Stress-strain curve:

Signature of the material and main tool for deriving its mechanical properties

\[ \sigma \]  
\[ \varepsilon \]

\[ A \] \[ B \] \[ C \] \[ D \]

\[ x = \text{failure} \]

If the curve is monotonic, a force-control is sufficient.

You can derive \( \widehat{AB} \) in displacement control, \( \widehat{CD} \) in crack-opening. The dashed area is the kinetic energy released per unit volume under displacement control.
Mechanical properties

\[ \frac{d\sigma}{d\varepsilon} \bigg|_0 \equiv E \equiv \text{Young's modulus} \]

\[ \sigma_{\text{max}} = \text{maximum stress} \equiv \text{Strength} \]

\[ \varepsilon_u = \text{ultimate strain} \]

\[ \int_0^{\varepsilon_u} \sigma d\varepsilon = \frac{\bar{E}}{V} = \text{Energy dissipated per unit volume or Toughness modulus.} \]

\[ \bar{E} = \int F \, dl \quad \quad V = Al \]

\[ \frac{\bar{E}}{V} = \int \frac{F \, dl}{A \, l} = \int \sigma d\varepsilon \]

The toughness modulus is a material property only for ductile materials.
Size-effects

The post-critical behaviour is size-dependent especially for brittle materials.

\[ l \to 0 \quad \text{ductile} \]

\[ l \to \infty \quad \text{brittle} \]
For brittle materials $\frac{\bar{E}}{V}$ has no meaning: instead of the toughness modulus we have to use the fracture energy.

\[
\bar{E} = G_c A
\]

$G_c \equiv$ fracture energy or energy dissipated per unit area

\[
\int \sigma d\varepsilon \equiv \frac{\bar{E}}{V} = \frac{G_c A}{lA} = \frac{G_c}{l}
\]

The reality is in between: energy dissipated on a fractal domain:

\[
\frac{\bar{E}}{V} \propto \bar{l}^{D-3} \quad \bar{l} = \frac{3}{\sqrt{V}}
\]

$D$ is the fractal exponent, $2 \leq D \leq 3$
Fracture Mechanics

\[ \sigma_{\text{tip}} \sim \frac{K_I}{\sqrt{2\pi r}} \]

\( K_I \equiv \text{Stress intensity factor} \)

Elastic solution is singular:
We cannot say
\[ \sigma_f: \sigma_{\text{tip}} = \sigma_{\text{max}} \]

\( \sigma_f \) stress at fracture
Linear Elastic Fracture Mechanics (LEFM)

Griffith’s approach

\[ G = -\frac{dW}{dA} \]

Energy release rate

\[ W = \bar{E} - L \]

Total potential energy

Crack surface area

External work

Stored elastic energy

Crack propagation criterion:

\[ G = G_c \]

\[ G = \frac{K_I}{E} \]

Elastic solution

\[ K_I = K_{IC} \]

Fracture toughness

\[ K_{IC} = \sqrt{G_c E} \]

\( G_c \equiv \) fracture energy

\( K_I \) only for a function of external load and geometry
$K_I$ values reported in stress-intensity factor Handbooks

E.g., infinite plate (i.e. width $\gg$ crack length $\sim$ graphene)

$$K_I = \sigma \sqrt{\pi a}$$

Strength of graphene with a crack of length $2a$

$$K_I = \sigma \sqrt{\pi a} = K_{IC}$$

$$\sigma_f = \frac{K_{IC}}{\sqrt{\pi a}}$$

Assuming statistically $a \propto \tilde{l} \equiv$ structural size:

$$\sigma_f \propto \tilde{l}^{-1/2}$$

Size effect on a fracture strength $\implies$ larger is weaker

problem of the scaling up….
With graphene pioneer Rod Ruoff we invented Quantized Fracture Mechanics (2004). The hypothesis of the continuous crack growth is removed: existence of fracture quanta due to the discrete nature of matter.
Related papers:


Quantized Fracture Mechanics (QFM)

\[ G^* = -\frac{\Delta W}{\Delta A} \]

Quantized energy release rate

\[ \Delta A = \text{fracture quantum of surface area} = qt \]

Fracture quantum of length

\[ G^* = G_C \]

Plate thickness

\[ G = -\frac{dW}{dA} \quad \Delta W = -\int GdA = -\int \frac{K_I^2}{E} dA \]

Quantized stress-intensity factor (generalized):

\[ G^* = -\frac{\Delta W}{\Delta A} = \frac{\int \frac{K_I^2}{E} dA}{\Delta A} \]

\[ G^* = G_C \quad \frac{1}{\Delta A} \int \frac{K_I^2}{E} dA = \frac{K_{IC}^2}{E} \]

\[ K_I^* = \sqrt{\frac{1}{\Delta A} \int K_I^2 dA} = K_{IC} \]
Monolayer graphene and examples


- Young’s modulus $E = 1$ TPa
- Intrinsic strength $\sigma_{\text{int}} = 130$ GPa
- Ultimate strain $\varepsilon_u = 25\%$

Monolayer graphene hanging on a silicon substrate (scale bar: 50µm)

Tensile test on macro samples of graphene composites

Tennis racket made of graphene (Head ©)
Carbon nanotubes


The singlewalled carbon nanotubes (SWCNTs) presents:
- Young’s modulus $\equiv E = 1000$ GPa
- Tensile strength $\sigma = 300$ GPa
- Ultimate strain $\varepsilon_u = 30\%$

The MWCNTs breaks in the outermost layer (“sword-in-sheath” failure),
- Young’s modulus $\equiv E = 250$ to 950 GPa
- Tensile strength $\sigma = 11$ to 63 GPa
- Ultimate strain $\varepsilon_u = 12\%$

Multiwalled carbon nanotubes (MWCNTs)
Exercise 1

E.g., infinite plate

\[ K_I = \sigma \sqrt{\pi a} \]

\[ K_I^* = \frac{1}{\sqrt{q t}} \int_a^{a+q} \sigma^2 \pi a t \, da = \sigma \frac{\pi}{2q} [(a + q)^2 - a^2] = \sigma \sqrt{\pi \left( a + \frac{q}{2} \right)} \]

Strength of graphene \( K_I^* = K_{IC} \)

\[ \sigma_f = \frac{K_{IC}}{\sqrt{\pi \left( a + \frac{q}{2} \right)}} \]

\( a \uparrow \quad \sigma_f \downarrow \) Unstable crack growth
$q \to 0 \quad \text{Correspondence Principle} \quad QFM \to LEFM$

$a \to 0 \quad \sigma_f = \sigma_{\text{ideal}}$

$$\sigma_{\text{ideal}} = \frac{K_{IC}}{\sqrt{\pi \frac{q}{2}}} \implies q = \frac{2}{\pi} \frac{K_{IC}^2}{\sigma_{\text{ideal}}^2}$$

Very close to predictions by MD and DFT

Very close to experimental measurement (2014)

$\sigma_{\text{ideal}} \sim 100 \text{ GPa}$

$\sigma_{\text{ideal}} \sim \frac{E}{10} \quad E \sim 1 \text{ TPa}$

Peeling of graphene

\[ E \to \infty \quad \bar{E} \to 0 \]

\[ \delta = l - l \cos \theta \]

\[ G = -\frac{dW}{dA} = \frac{dL}{dA} \quad L = Fd \quad dA = bdl \]

\[ G = \frac{d}{bdl} Fl(1 - \cos \theta) = \frac{F(1 - \cos \theta)}{b} \]

\[ G = G_C \quad \implies \quad F_C = \frac{bG_C}{1 - \cos \theta} \]

\( F_C \) strongly dependent on \( \theta \)

Exercise 3

Apply LEFM for measuring the fracture toughness of a sheet of paper with a crack of a certain length in the middle:
Bending theory

Bending of beams

\[ \frac{d\varphi_x}{2} \approx y \frac{d\varphi_x}{2} \]

\[ \frac{\varepsilon dz}{2} \approx y \frac{d\varphi_x}{2} \]

\[ \frac{M_x}{I_x} y \approx K y \]

\[ M_x = \int_{-h/2}^{h/2} \sigma_z y b dy = K I_x \]

\[ \chi_x = \frac{1}{R_x} = \frac{d\varphi_x}{dz} = \frac{\varepsilon_z}{y} = \frac{\sigma_z}{Ey} = \frac{M_x}{I_x E} \]

\[ \chi_{\text{max}} = \frac{\varepsilon_{z,\text{max}}}{h/2} \]
Exercise 4

Derive the maximal graphene curvature.

For graphene \( h = t \approx 0.34 \, \text{nm} \rightarrow \chi_{\text{max}} \text{huge} \rightarrow \) flexibility is more a structural than a material property

\[
\varphi_x = -\frac{dv}{dz} \Rightarrow \frac{d^2 v}{dz^2} = -\frac{M_x}{I_x E}
\]

Load per unit length

\[
\frac{dT}{dz} = -q \quad \Rightarrow \quad \frac{d^4 v}{dz^4} = \frac{q}{I_x E}
\]

Elastic line equation

Load per unit area

\[
\nabla^4 W = \frac{q}{D}
\]

Elastic plane equation

Bending stiffness

\[
D = \frac{E t^3}{12(1 - \nu^2)}
\]