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MECHANICS OF 2D MATERIALS

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Outline

- Stretching
  - Stress } Stress-Strain curve
  - Strain }
- 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

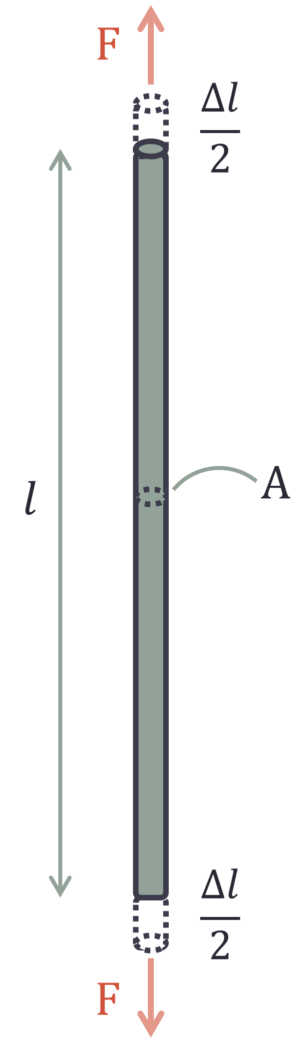
1. Apply LEFM for measuring the fracture toughness of a sheet of paper;
2. Apply the Bending theory for calculating the maximal curvature before fracture.

Stretching

Fiber under tension

Stress: $\sigma = \frac{F}{A}$

Strain: $\varepsilon = \frac{\Delta l}{l}$



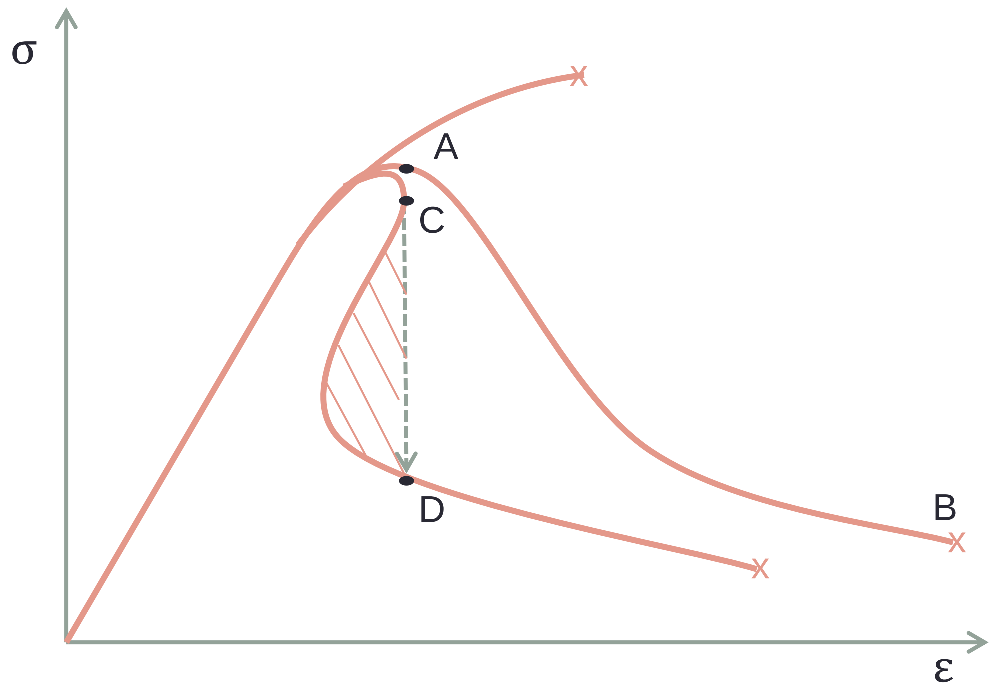
Stress-strain curve:

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

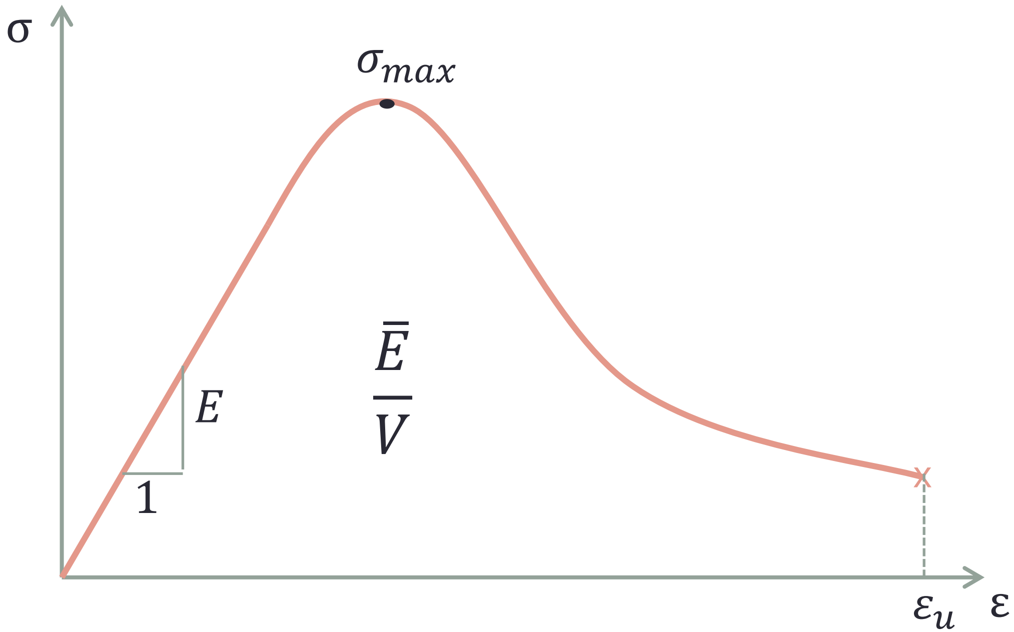
x = failure

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

You can derive $\overset{\frown}{AB}$ in displacement control, $\overset{\frown}{CD}$ in crack-opening. The dashed area is the kinetic energy released per unit volume under displacement control.



Mechanical properties



$\left.\frac{d\sigma}{d\varepsilon}\right|_0 \equiv E \equiv$ Young's modulus

σ_{max} = maximum stress ≡ Strength

ε_u = ultimate strain

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

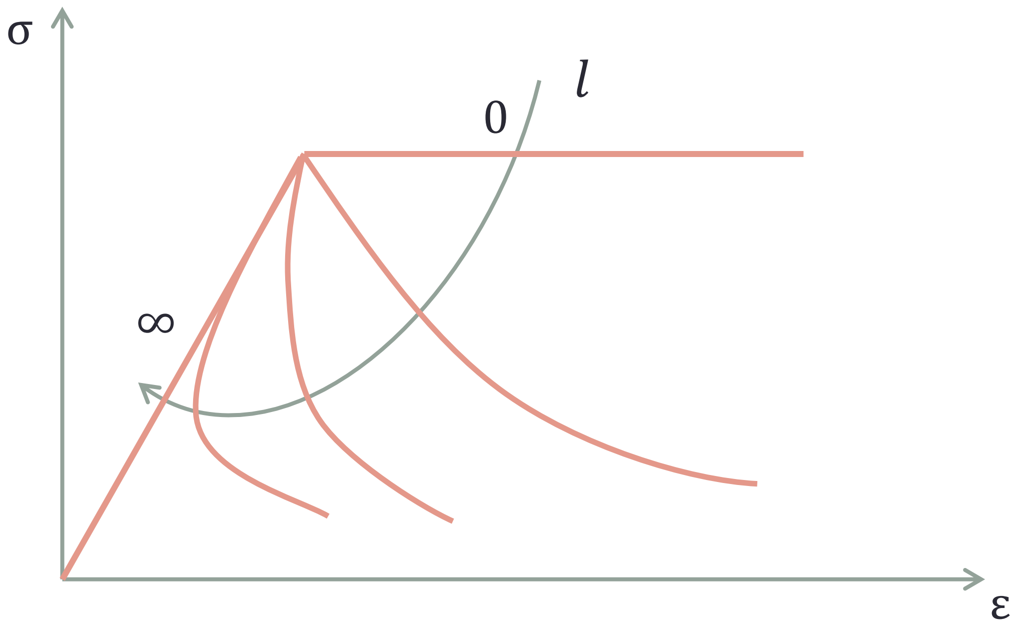
$$\bar{E} = \int F dl \qquad V = Al$$

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

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

Size-effects

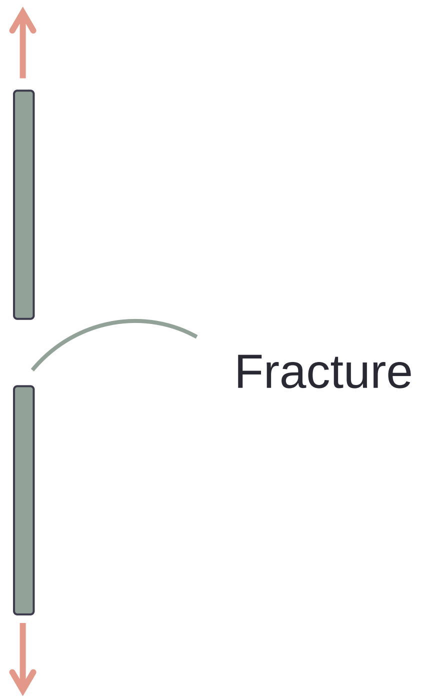
The post-critical behaviour is size-dependent especially for brittle materials.



$l \to 0$ ductile

$l \to \infty$ 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

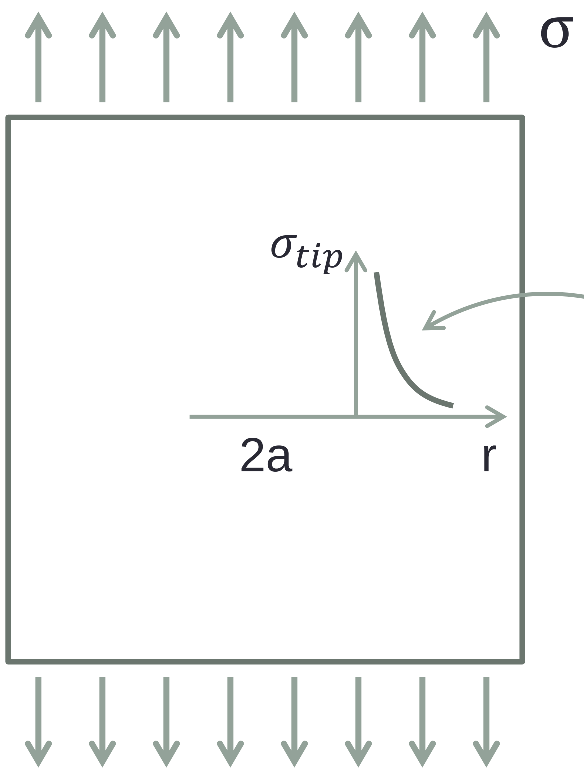
$$\int \sigma d\varepsilon \equiv \frac{\bar{E}}{V} = \frac{G_c A}{lA} = \frac{G_c}{l}$$

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

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

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

Fracture Mechanics



$K_I \equiv$ Stress intensity factor

constant

$$\sigma_{tip} \sim \frac{K_I}{\sqrt{2\pi r}}$$

Elastic solution is singular:
We cannot say

$$\sigma_f : \sigma_{tip} = \sigma_{max}$$

σ_f stress at fracture

Linear Elastic Fracture Mechanics (LEFM)

Griffith's approach

$$G = -\frac{dW}{dA}$$

Energy release rate → G

Crack surface area → dA

$$W = \bar{E} - L$$

Total potential energy → W

Stored elastic energy → $\bar{E}$

External work → L

Crack propagation criterion:

$$\boldsymbol{G = G_C}$$

$G_c \equiv$ fracture energy

$G = \frac{K_I}{E}$ Elastic solution

K_I only for a function of external load and geometry

$$\boldsymbol{K_I = K_{IC}}$$

$K_{IC} = \sqrt{G_C E}$ Fracture toughness

K_I values reported in stress-intensity factor Handbooks

E.g., infinite plate (i.e. width $\gg$ crack length ~ 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 ⇨ larger is weaker

⇨ problem of the scaling up….

Paradox $\sigma_f \to \infty \quad a \to 0$

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.

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Quantized fracture mechanics

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ABSTRACT

A new energy-based theory, quantized fracture mechanics (QFM), is presented that modifies continuum-based fracture mechanics; stress- and strain-based QFM analogs are also proposed. The differentials in Griffith's criterion

Related papers:

N. M. Pugno, “*Dynamic quantized fracture mechanics*”, Int. J. Fract, 2006

N. M. Pugno, “*New quantized failure criteria: application to nanotubes and nanowires*”, Int. J. Fract, 2006

Quantized Fracture Mechanics (QFM)

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

↑ Quantized energy release rate

ΔA = fracture quantum of surface area = qt

q: Fracture quantum of length; t: Plate thickness

$$G^* = G_C$$

$$G = -\frac{dW}{dA} \qquad \Delta W = -\int G dA = -\int \frac{{K_I}^2}{E} dA$$

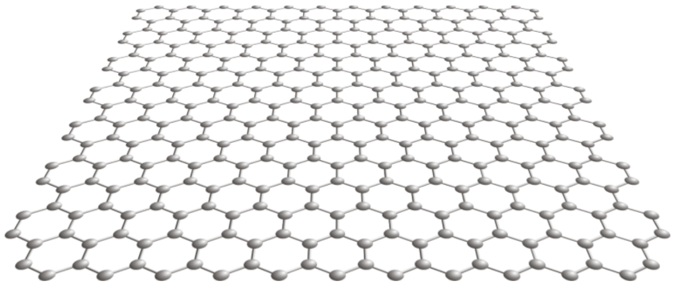
$$G^* = -\frac{\Delta W}{\Delta A} = \frac{\int \frac{{K_I}^2}{E} dA}{\Delta A} \qquad G^* = G_c \qquad \frac{1}{\Delta A}\int \frac{{K_I}^2}{E} dA = \frac{{K_{IC}}^2}{E}$$

Quantized stress-intensity factor (generalized):

$$K_I^* = \sqrt{\frac{1}{\Delta A}\int {K_I}^2\, dA} = K_{IC}$$

Monolayer graphene and examples

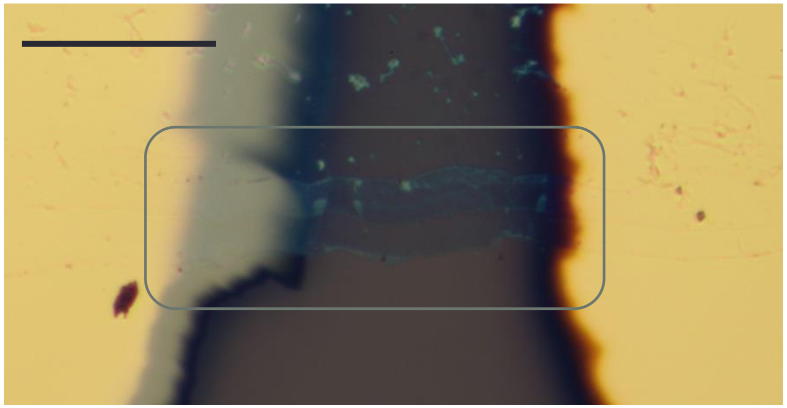
C. Lee, X. Wei, J.W. Kysar, J. Hone,
"*Measurement of the elastic properties and intrinsic strength of monolayer graphene*", Science, 2008 :



Young's modulus $\equiv E = 1$ TPa

Intrinsic strength $\sigma_{int} = 130$ GPa

Ultimate strain $\varepsilon_u = 25$ %



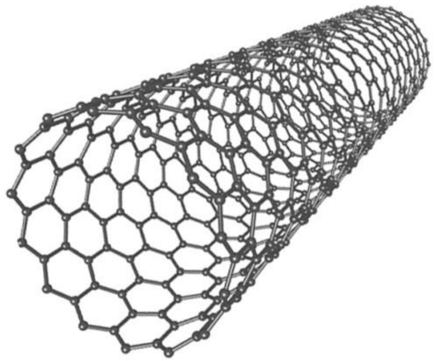
Monolayer graphene hanging on a silicon substrate (scale bar: 50µm)

Tensile test on macro samples of graphene composites

Tennis racket made of graphene (*Head* ©)

Carbon nanotubes

Min-Feng Yu, Oleg Lourie, Mark J. Dyer, Katerina Moloni, Thomas F. Kelly, Rodney S. Ruoff, "*Strength and Breaking Mechanism of Multiwalled Carbon Nanotubes Under Tensile Load*", Science, 2000:

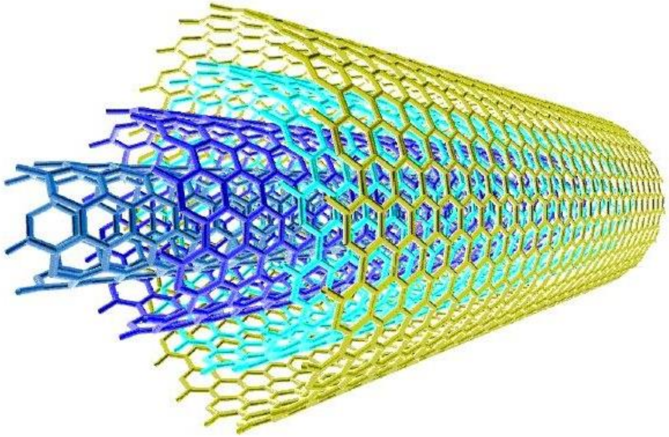


The singlewalled carbon nanotubes (SWCNTs) presents:

Young's modulus ≡ E =1000 GPa

Tensile strength σ = 300 GPa

Ultimate strain $\varepsilon_u = 30\ \%$



Multiwalled carbon nanotubes (MWCNTs)

The MWCNTs breaks in the outermost layer ("sword-in-sheath" failure),

Young's modulus ≡ E =250 to 950 GPa

Tensile strength σ = 11 to 63 GPa

Ultimate strain $\varepsilon_u = 12\ \%$

Exercise 1

E.g., infinite plate

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

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

Strength of graphene $K_I{}^* = K_{IC}$

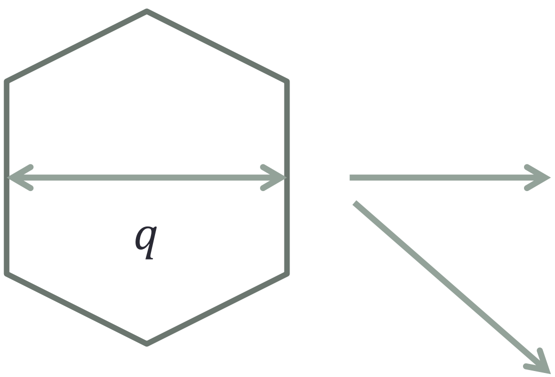
$$\sigma_f = \frac{K_{IC}}{\sqrt{\pi\left(a+\frac{q}{2}\right)}}$$

$a \uparrow \quad \sigma_f \downarrow$ Unstable crack growth

$q \to 0$ Correspondence Principle $QFM \to LEFM$

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

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



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

Very close to predictions by MD and DFT

$K_{IC} \sim 3\text{MPa}\sqrt{\text{m}}$

(QFM 2004)

Very close to experimental measurement (2014)

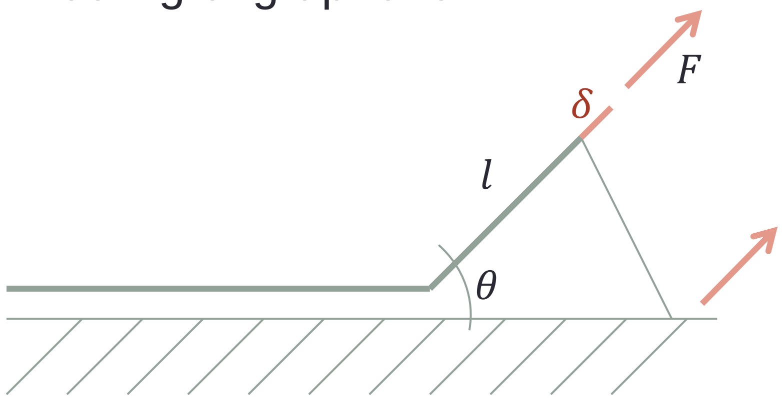
$\sigma_{ideal} \sim 100 \text{ GPa}$

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

P. Zhang, L. Ma, F. Fan, Z. Zeng, C. Peng, P. E. Loya, Z. Liu, Y. Gong, J. Zhang, X. Zhang, P. M. Ajayan, T. Zhu & J. Lou, *Fracture toughness of graphene,* Nature, 2014

Exercise 2

Peeling of graphene



$$E \to \infty \qquad \bar{E} \to 0$$

$$\delta = l - l\cos\theta$$

$$G = -\frac{dW}{dA} = \frac{dL}{dA} \qquad L = Fd \qquad dA = bdl$$

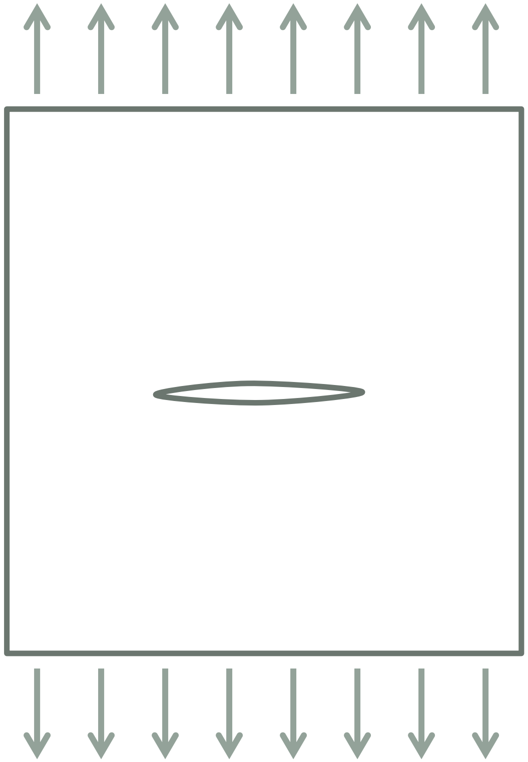
$$G = \frac{d}{bdl} Fl(1 - \cos\theta) = \frac{F(1 - \cos\theta)}{b}$$

$$G = G_C \quad \Longrightarrow \quad F_C = \frac{bG_C}{1 - \cos\theta}$$

F_C strongly dependent on θ

N. M. Pugno, "*The theory of multiple peeling*", Int. J. Fract, 2011

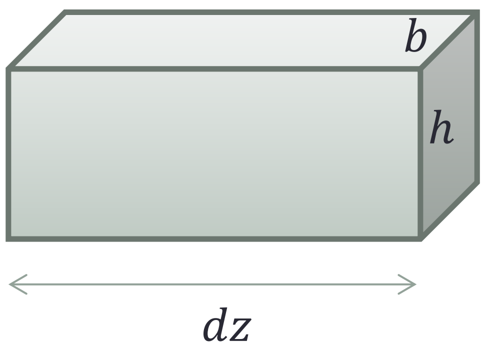
Exercise 3

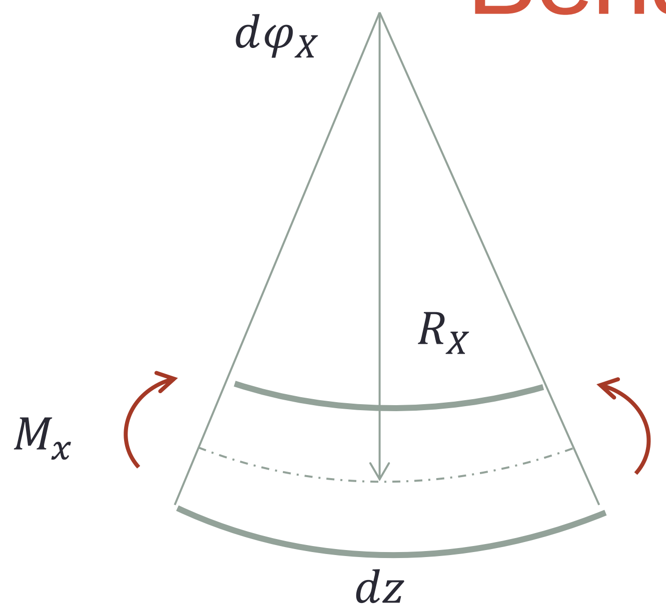


Apply LEFM for measuring the fracture toughness of a sheet of paper with a crack of a certain length in the middle:

Bending theory

Bending of beams

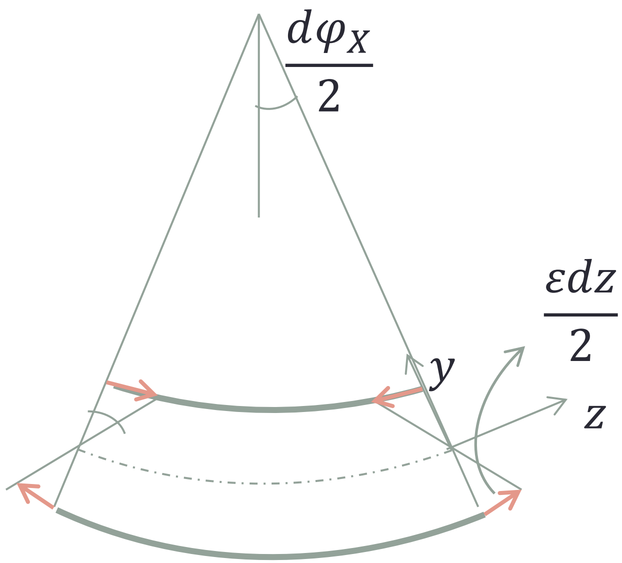




Bending Moment

Moment of inertia

$$I_x = \frac{bh^3}{12}$$



$$\frac{\varepsilon dz}{2} \cong y\frac{d\varphi_X}{2}$$

$$\sigma_z = \frac{M_x}{I_x}y \cong Ky \qquad M_x = \int_{-\frac{h}{2}}^{\frac{h}{2}} \sigma_z y b dy = KI_x$$

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

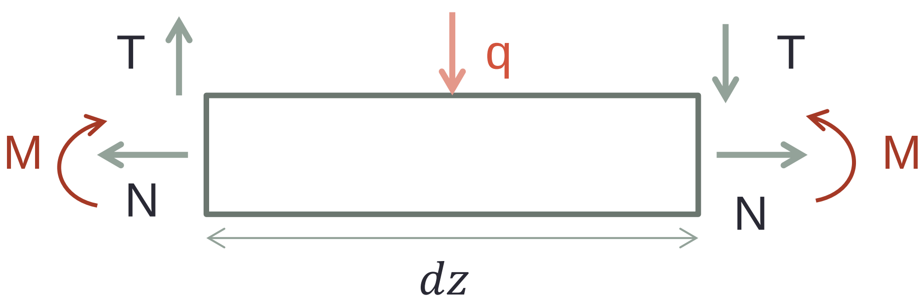
$$\chi_{max} = \frac{\varepsilon_{z,max}}{h/2}$$

Exercise 4

Derive the maximal graphene curvature.

For graphene $h = t \cong 0.34\ nm$ $\rightarrow \chi_{max}$huge → flexibility is more a structural than a material property

$$\varphi_x = -\frac{dv}{dz} \Longrightarrow \frac{d^2v}{dz^2} = -\frac{M_x}{I_x E}$$



Load per unit length

$$\left.\begin{aligned} \frac{dT}{dz} &= -q \\ \frac{dM}{dz} &= T \end{aligned}\right\} \Longrightarrow \boxed{\frac{d^4v}{dz^4} = \frac{q}{I_x E}}$$

Elastic line equation

For plates: $\nabla^4 W = \frac{q}{D}$

Load per unit area

Elastic plane equation

Bending stiffness $D = \dfrac{Et^3}{12(1-\nu^2)}$