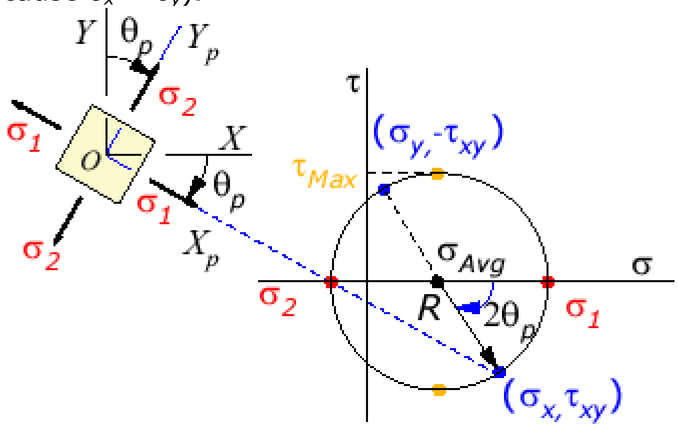
PROBLEM SET 7
DUE FRIDAY NOVEMBER 7th

MOHR'S CIRCLE

1. Given a plane with stresses σ_x and σ_y and τ_{xy}, draw the Mohr's circle if the plane rotates 45º clockwise to the current axes. Hint: **$\tau_{xy} < 0$ and $\sigma_x > \sigma_y$**
2. Given a plane with stresses σ_x and σ_y and τ_{xy}, draw the Mohr's circle if the plane rotates counterclockwise to the current axes between 45-90degrees.
   Hint: **$\tau_{xy} > 0$ and $\sigma_x < \sigma_y$**
3. Given a plane with stresses σ_x and σ_y and τ_{xy}, draw the Mohr's circle if the plane rotates 45º clockwise to the current axes between 45-90 degrees. Hint: **$\tau_{xy} < 0$ and $\sigma_x < \sigma_y$**
4. Given a plane with stresses σ_x and σ_y and τ_{xy}, draw the Mohr's circle if the principle axes are aligned with current axes. Hint: **$\tau_{xy} = 0$ and $\sigma_x > \sigma_y$**

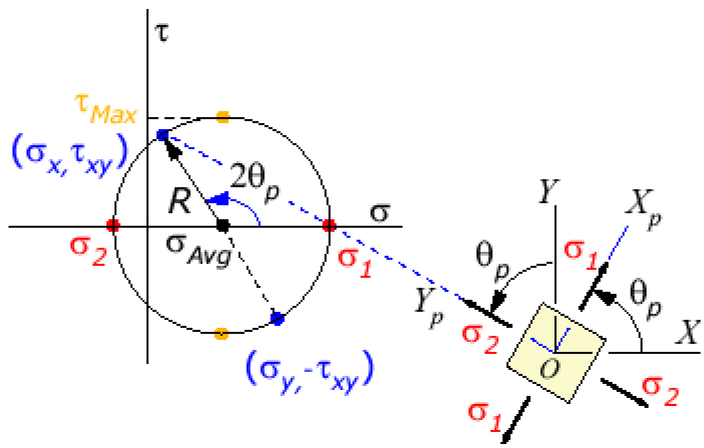
Problem #1: $\tau_{xy} < 0$ and $\sigma_x > \sigma_y$

The principal axes are clockwise to the current axes (because $\tau_{xy} < 0$) and no more than 45º away (because $\sigma_x > \sigma_y$).



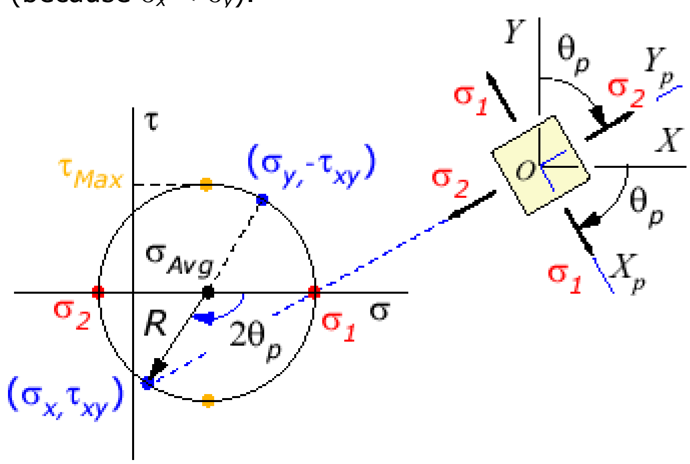
Problem #2: $\tau_{xy} > 0$ and $\sigma_x < \sigma_y$

The principal axes are counterclockwise to the current axes (because $\tau_{xy} > 0$) and between 45º and 90º away (because $\sigma_x < \sigma_y$).



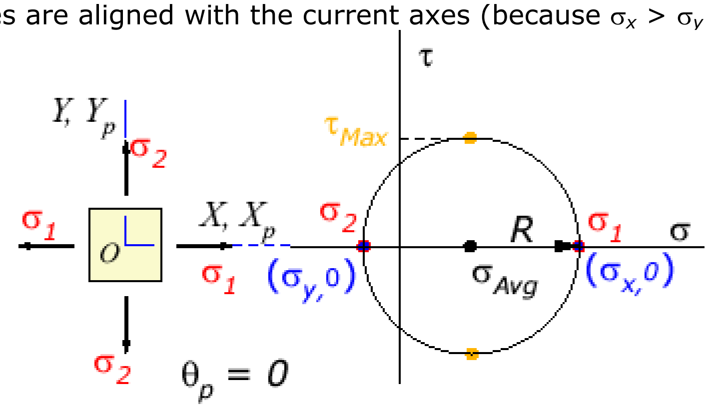
Problem #3: $\tau_{xy} < 0$ and $\sigma_x < \sigma_y$

The principal axes are clockwise to the current axes (because $\tau_{xy} < 0$) and between 45º and 90º away (because $\sigma_x < \sigma_y$).



Problem #4: $\tau_{xy} = 0$ and $\sigma_x > \sigma_y$

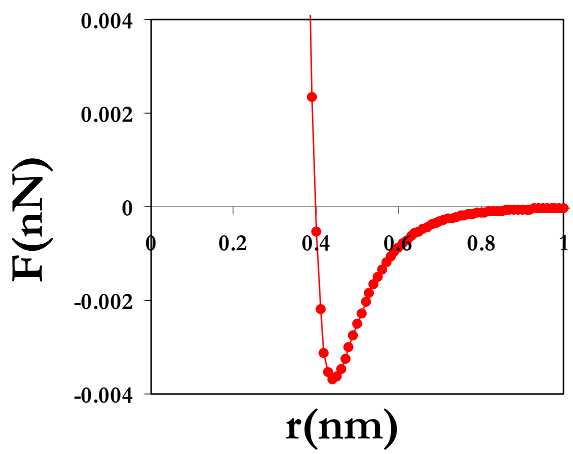
The principal axes are aligned with the current axes (because $\sigma_x > \sigma_y$ and $\tau_{xy} = 0$).



LENNARD-JONES POTENTIAL

Problem #5

Two atoms interact at T=0ºK via a van der Waals Lennard-Jones potential with A=4.7•10^{-78} Jm^{6}. The interaction force versus separation distance plot is given in the

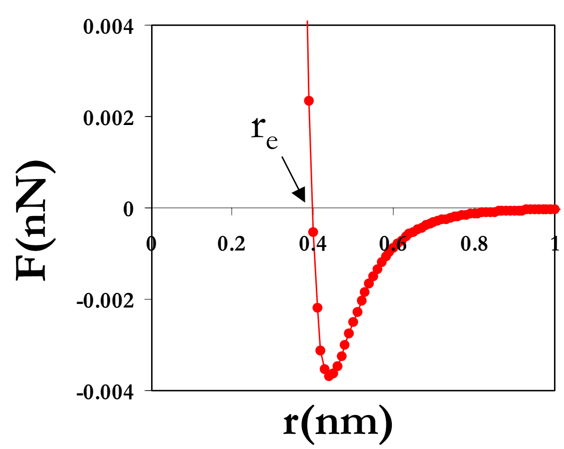


following figure.

(a) Calculate the binding energy (k_BT) and the bond stiffness (N/m).

(b) The two atoms are held at a particular separation distance r using an atomic force microscope so that the *attractive component* of the force is equal to -0.003 nN. At this distance are the atoms attracted to each other or repelled away from each other ? Justify your answer with a numerical calculation.

A. (a) the equilibrium bond length, r_e, can be read directly off the plot as the separation distance where the $F(r_e)=0 \Rightarrow r_e=0.4$ nm.



$r_e=[2B/A]^{1/6}$ *(1)*
Solve equation *(1)* for : $B=Ar_e^6/2$ *(2)*
Substitute in equation *(2)* known values for r_e and A :
$B=(4.7\bullet10^{-78}Jm^6)(0.4\bullet10^{-9}m)^6/2=10^{-134}Jm^{12}$

$E_B=-[A^2/4B]=-[(4.7\bullet10^{-77}Jm^6)^2/4\bullet10^{-134}Jm^{12}]=-5.522\bullet10^{-22}J\bullet k_BT/4.1\bullet10^{-21}J$
$E_B=-0.135k_BT$

$k_{bond}=42A/r_e^8-156B/r_e^{14}=42\bullet4.7\bullet10^{-77}Jm^6/(0.4\bullet10^{-9})^8-156\bullet10^{-134}Jm^{12}/(0.4\bullet10^{-9})^{14}$
$k_{bond}=0.3$ N/m

(b) $F=-6A/r^7+12B/r^{13}$
$F_{attractive}=-6A/r^7$ *(3)*
$F_{repulsive}=12B/r^{13}$ *(4)*

Solve equation *(3)* for r $\Rightarrow$ $r=[-6A/-F_{attractive}]^{1/7}$
$r=[-6\bullet4.7\bullet10^{-77}Jm^6/-0.003\bullet10^{-9}N]^{1/7}=0.5$ nm

Substitute r and B into equation *(4)* $\Rightarrow$ $F_{repulsive}=12\bullet10^{-134}Jm^{12}/(0.5\bullet10^{-9}m)^{13}$
$F_{repulsive}=0.0009$ nN

$F_{net}=F_{attractive}+F_{repulsive}=-0.003$ nN$+0.0009$ nN
$F_{net}=-0.00262$
[NET FORCE IS ATTRACTIVE]

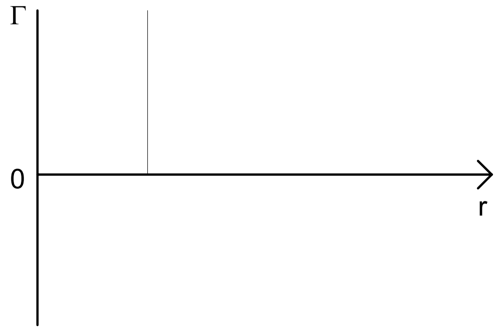
1) <u>Ideal Gas</u>

$$\Gamma(r)=0$$

2) <u>Hard Sphere</u>

$$\Gamma(r) = \infty \; (r \le \sigma)$$

$$\Gamma(r) = 0 \; (r > \sigma)$$



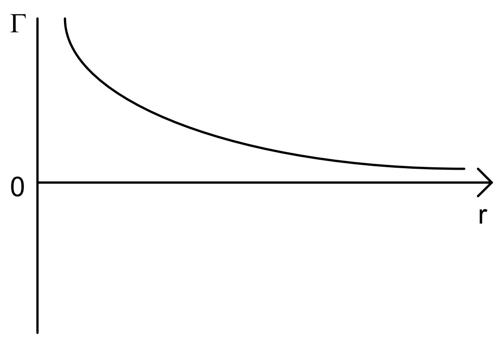
3) Point Repulsion

$$\Gamma(r) = dr^{-\delta}$$

δ = index of repulsion;

$$9 < \delta < 15$$

If $\delta = 4 \Rightarrow$ "Maxwellian molecules"

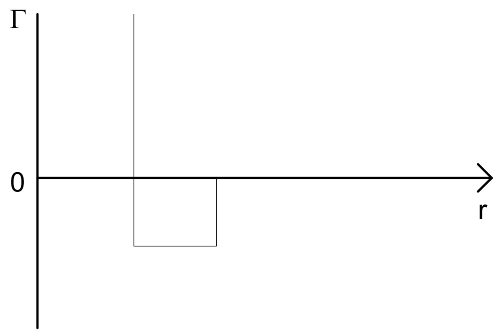


4) Square Well

$$\Gamma(r) = \infty \quad (r \le \sigma)$$

$$\Gamma(r) = -\varepsilon \quad (\sigma < r \le R\sigma)$$

$$\Gamma(r) = 0 \quad (r > R\sigma)$$

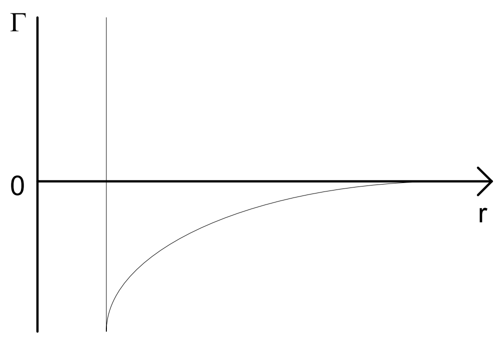


5) <u>Sutherland</u>

$$\Gamma(r) = \infty \quad (r \le \sigma)$$

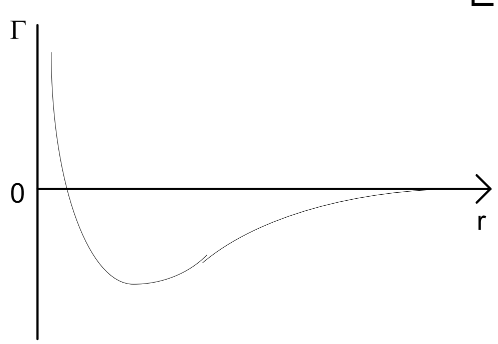
$$\Gamma(r) = -cr^{-\gamma} \quad (r > \sigma)$$

Typically, $\gamma = 6$



6) <u>Lennard-Jones</u>

$$\Gamma(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$



7) <u>Buckingham</u>

$$\Gamma(r) = b\exp(-ar) - \frac{c}{r^6} - \frac{c'}{r^8}$$

- 4-parameter
- exponential form for repulsive (theoretically better)
- includes induced dipole / induced dipole & induced dipole / induced quadrupole

- numerically difficult
  - goes to $-\infty$ at $r = 0$ [**UNREALISTIC** !!]