# Lecture 8

# Introduction to Contact Mechanics

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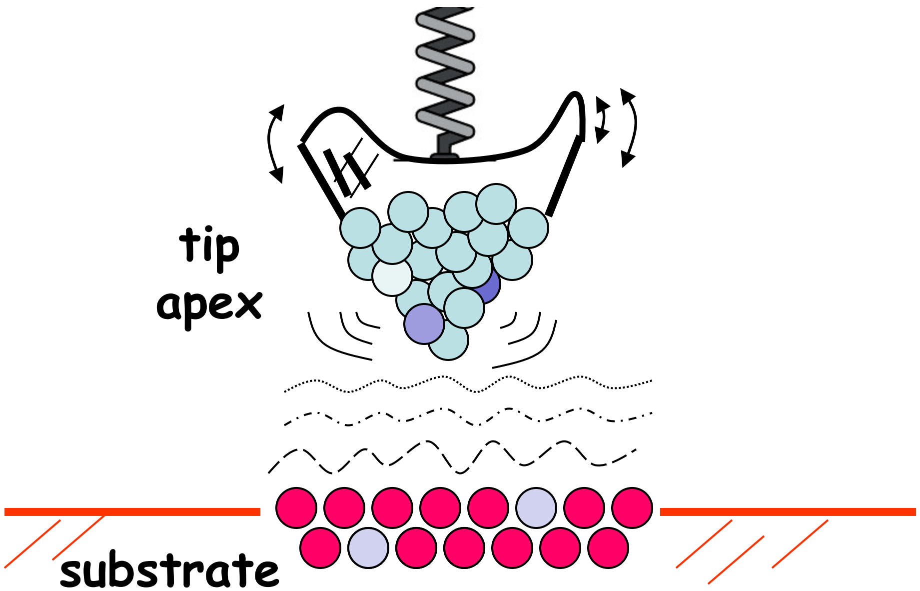
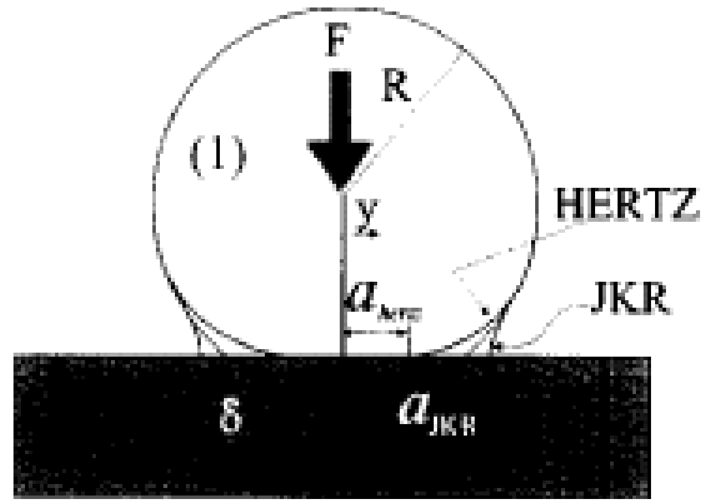
# How to Model the Repulsive Interaction at Contact?

## Atom-Atom?




## Sphere-Plane?




Source: Capella & Dietler

Maybe if the contact area involves tens or hundreds of atoms the description of net repulsive force is best captured by continuum elasticity models

# What we want to know

Nature of the contact - reversible (elastic)? hysteretic?

Contact radius (contact area) as function of applied force

Any deformation?

Pull-off force (adhesion force)

What determines all these quantities?

# Continuum description of contact - history

- Hertz (1881) takes into account neither surface forces nor adhesion, and assumes a linearly elastic sphere indenting an elastic surface
- Sneddon's analysis (1965) considers a rigid sphere (or other rigid shapes) on a linearly elastic half-space.
- Neither Hertz or Sneddon consider surface forces discussed in last lecture.
- Bradley's analysis (1932) considers two <u>rigid</u> spheres interacting *via* the Lennard-Jones 6-12 potential
- Derjaguin-Müller-Toporov (DMT, 1975) considers an elastic sphere with rigid surface but includes van der Waals forces outside the contact region. Applicable to stiff samples with low adhesion.
- Johnson-Kendall-Roberts (JKR, 1971) neglects long-range interactions o utside contact area but includes short-range forces in the contact area. Applicable to soft samples with high adhesion.
- Maugis (1992) theory is even more accurate – shows that JKR and DMT are limits of same theory

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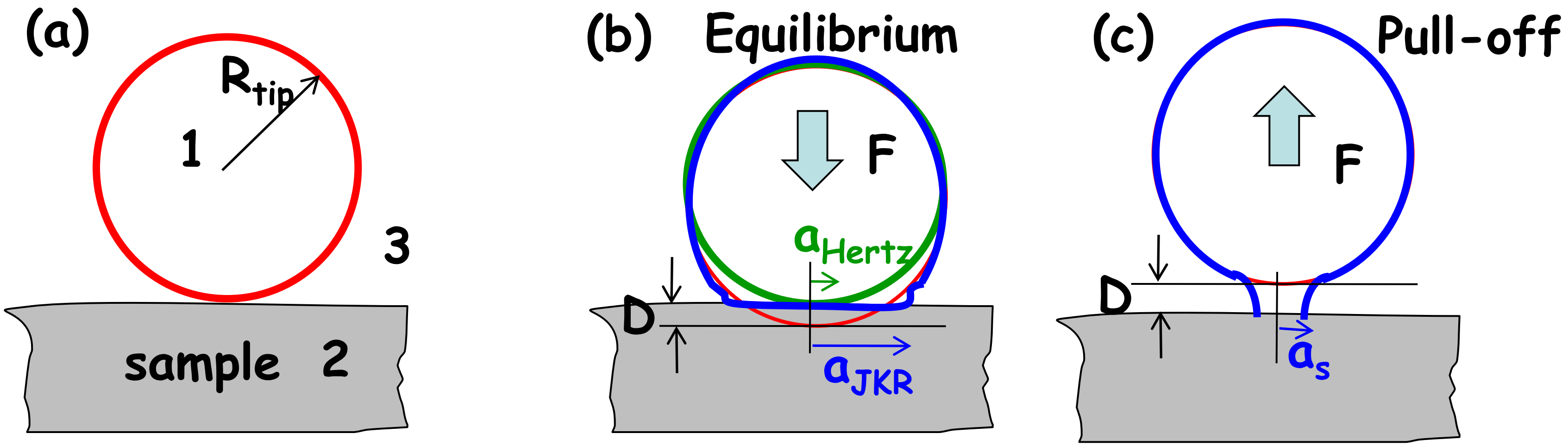
# Tip-sample Interaction Models




Rigid tip-rigid sample

Deformable tip and rigid sample*

- From the Derjaguin approximation for rigid tip interacting with rigid sample we have

$$F_{tip-sample}(r^*) = F_{adhesion} = 2\pi R_{tip} U(r^*) \simeq 2\pi R_{tip} W_{132} = 2\pi R_{tip}(\gamma_{13} + \gamma_{23} - \gamma_{12})$$

- Real tips and samples are **not** rigid. Several theories are used to better account for this fact (Hertz, DMT, JKR)
- * These theories also apply to elastic samples, they are just shown on rigid sample to demonstrate key quantities clearly. For example D is the **combined** tip-sample deformation in (b)

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# I. Surface energies - notation

- Work of adhesion and cohesion: work done to separate unit areas of two media 1 and 2 from contact to infinity in vacuum. If 1 and 2 are different then $W_{12}$ is the work of adhesion; if 1 and 2 are the same then $W_{11}$ is the work of cohesion. Think vdW's whenever you see work of adhesion/cohesion.
- Surface energy: This is the free energy change $\gamma$ when the surface area of a medium is increased by unit area. Thus

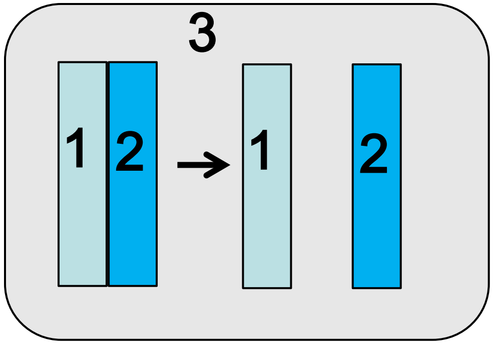
$$W_{11} = 2\gamma_1$$

- While separating dissimilar materials the free energy change in producing an "interfacial" $\gamma_{12}$ area by unit area is known as their interfacial energy

$$W_{12} = \gamma_1 + \gamma_2 - \gamma_{12}$$

- Work of adhesion in a third medium

$$W_{132} = \gamma_{13} + \gamma_{23} - \gamma_{12}$$

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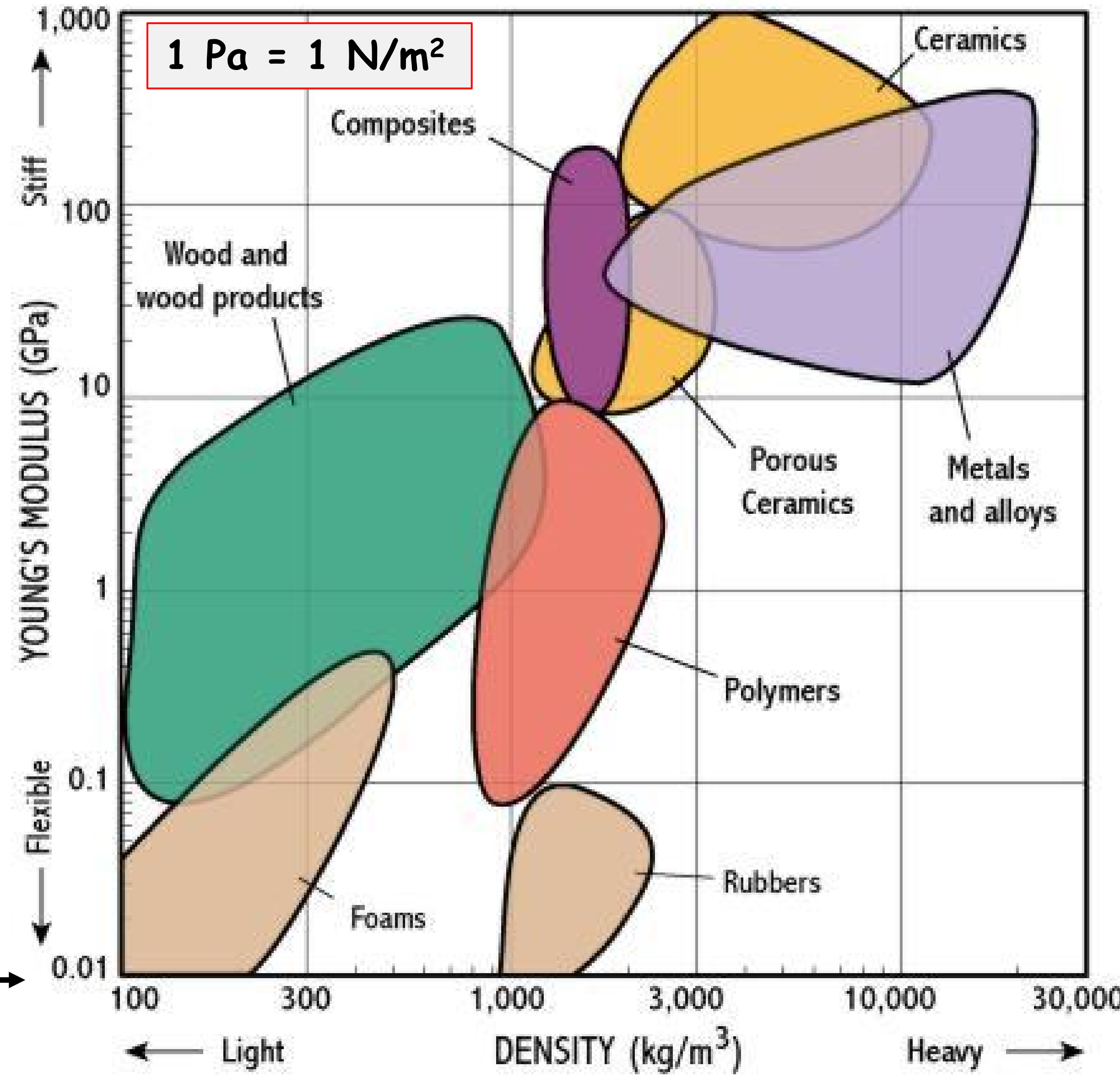
# II. What is the "Stiffness" of the Tip/Substrate?




10 MPa ⟷

five orders of magnitude

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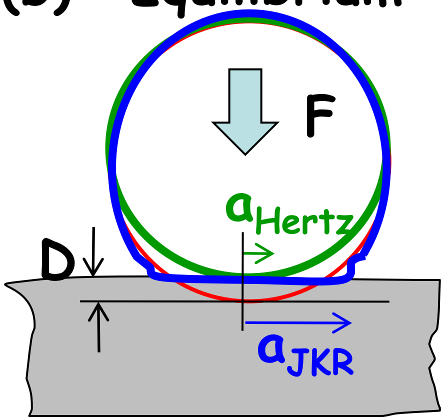
http://www-materials.eng.cam.ac.uk/mpsite/interactive_charts/stiffness-density/NS6Chart.html

# Standard results

(b) Equilibrium




**Contact radius a:**

$$a_{Hertz} = \left(\frac{R_{tip}F}{E_{tot}}\right)^{1/3} \qquad a_{DMT} = \left(\frac{R_{tip}(F + 2\pi R_{tip}W_{132})}{E_{tot}}\right)^{1/3}$$

$$a_{JKR} = \left(\frac{R_{tip}\left(F + 2\pi R_{tip}W_{132} + \sqrt{6\pi R_{tip}W_{132}F + (3\pi R_{tip}W_{132})^2}\right)}{E_{tot}}\right)^{1/3}$$

**Deformation D:**

$$D_{Hertz} = \frac{a^2}{R_{tip}} = \left(\frac{F^2}{R_{tip}E_{tot}{}^2}\right)^{1/3} \qquad D_{DMT} = \frac{a^2}{R_{tip}} = \left(\frac{\left(F + 2\pi R_{tip}W_{132}\right)^2}{R_{tip}E_{tot}{}^2}\right)^{1/3}$$

$$D_{JKR} = \frac{a^2}{R_{tip}} - \frac{2}{3}\sqrt{\frac{6\pi W_{132}a}{E_{tot}}}$$

$$\frac{1}{E_{tot}} = \frac{3}{4}\left(\frac{1-\nu_s{}^2}{E_s} + \frac{1-\nu_t{}^2}{E_t}\right) = \frac{3}{4}\frac{1}{E^*}$$

*sometimes* $E_{tot} = \frac{4}{3}E^*$

Source: Butt, Cappella, Kappl

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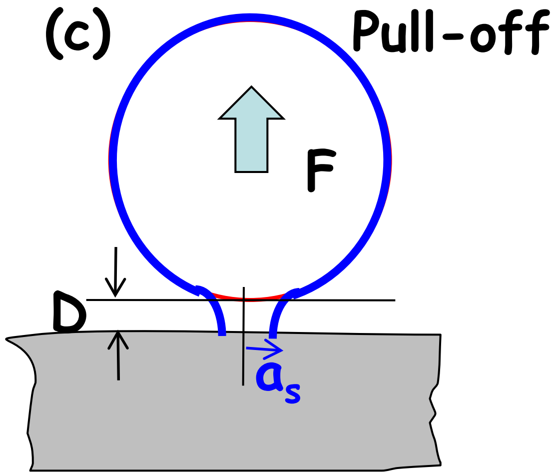
# Standard results (cont.)




**Pull-off Force F:**

$$F_{adhesion}^{Hertz} = 0$$

$$F_{adhesion}^{DMT} = 2\pi R_{tip} W_{132}$$

$$F_{adhesion}^{JKR} = \frac{3\pi}{2} R_{tip} W_{132}$$

Source: Butt, Cappella, Kappl

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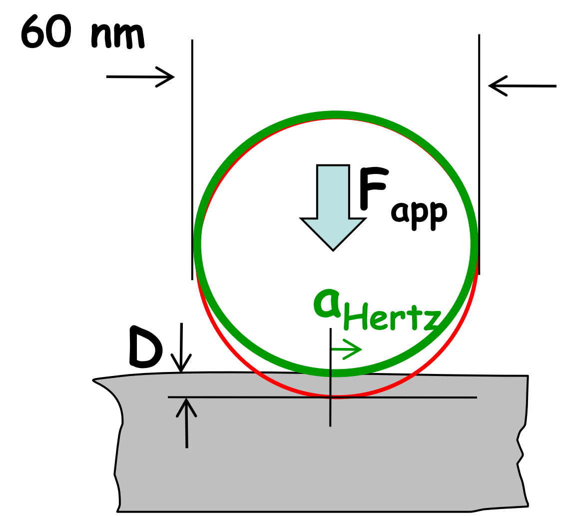
# Example

**Hertz contact:** $R_{tip}$ = 30 nm; $F_{app}$= 1 nN

$E_{tip}=E_{sub}$=200 Gpa; Poisson ratio = $v_{tip}=v_{sub}=0.3=v$

$$\frac{1}{E_{tot}} = \frac{3}{4}\left(\frac{1-\nu_{sub}^{2}}{E_{sub}} + \frac{1-\nu_{tip}^{2}}{E_{tip}}\right) = \frac{3}{2}\frac{1-\nu^{2}}{E}$$

$$= \frac{3}{2}\frac{0.91}{(200GPa)} = \frac{1.365}{200GPa} \Rightarrow \quad E_{tot} = 146.5GPa$$




**Contact radius:**

$$a_{Hertz} = \left(\frac{R_{tip}F}{E_{tot}}\right)^{1/3} = 0.59\ nm$$

**Deformation:**

$$D_{Hertz} = \frac{a^{2}}{R_{tip}} = \left(\frac{F^{2}}{R_{tip}E_{tot}^{2}}\right)^{1/3} = 12\ pm$$

**Pull-off Force=0**

**Contact Pressure:** $$P \simeq \frac{F}{\pi a_{Hertz}^{2}} = 0.9\,GPa \approx 9000\ atmos.$$

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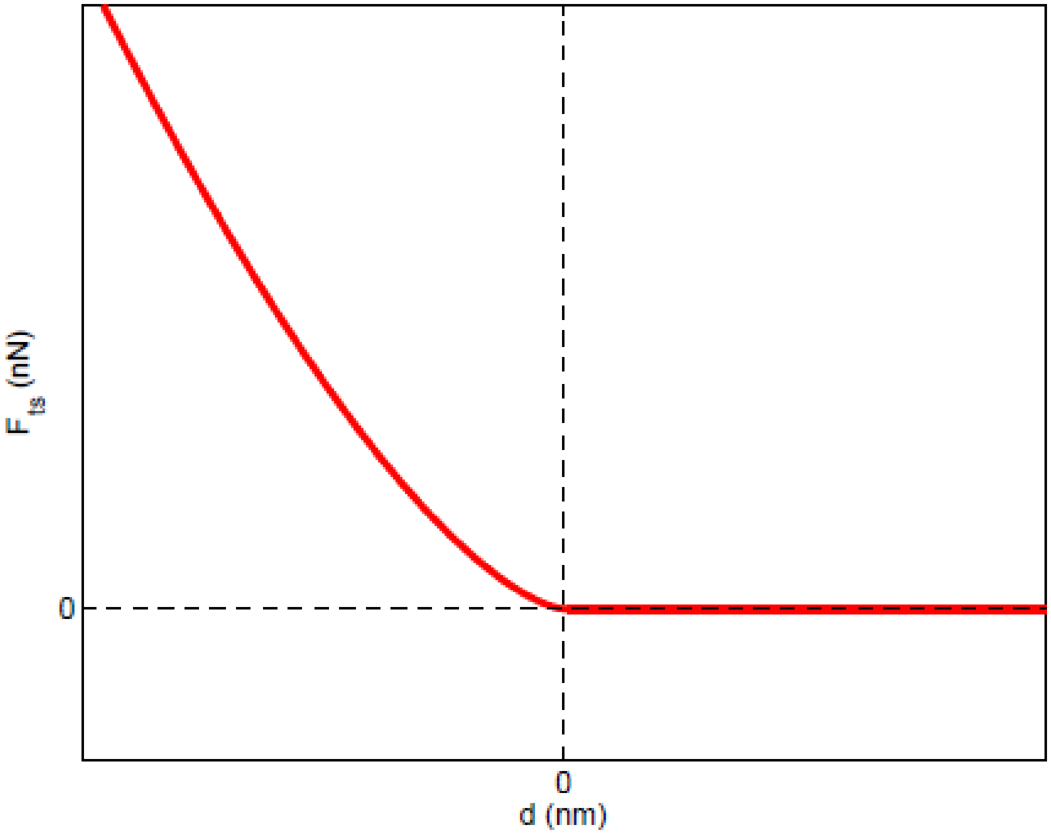
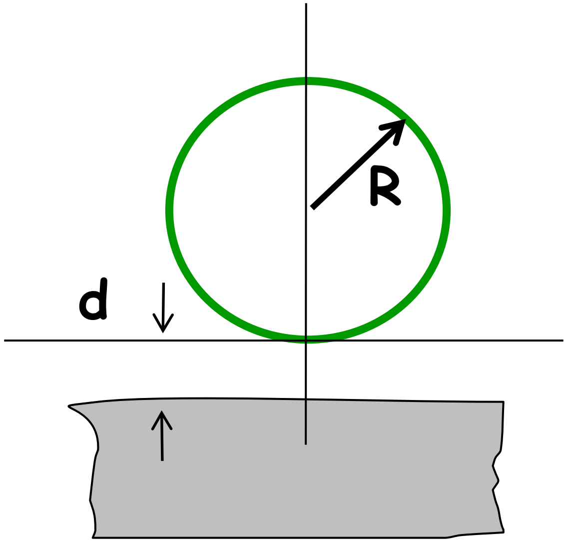
# Hertz




$$F_{ts}(d) = \begin{cases} 0, & d > 0 \\ \frac{4}{3} E^* \sqrt{R} (-d)^{3/2}, & d \leq 0 \end{cases}$$

$$E^* = \left[ \frac{1 - \nu_{tip}^2}{E_{tip}} + \frac{1 - \nu_{sample}^2}{E_{sample}} \right]^{-1}$$

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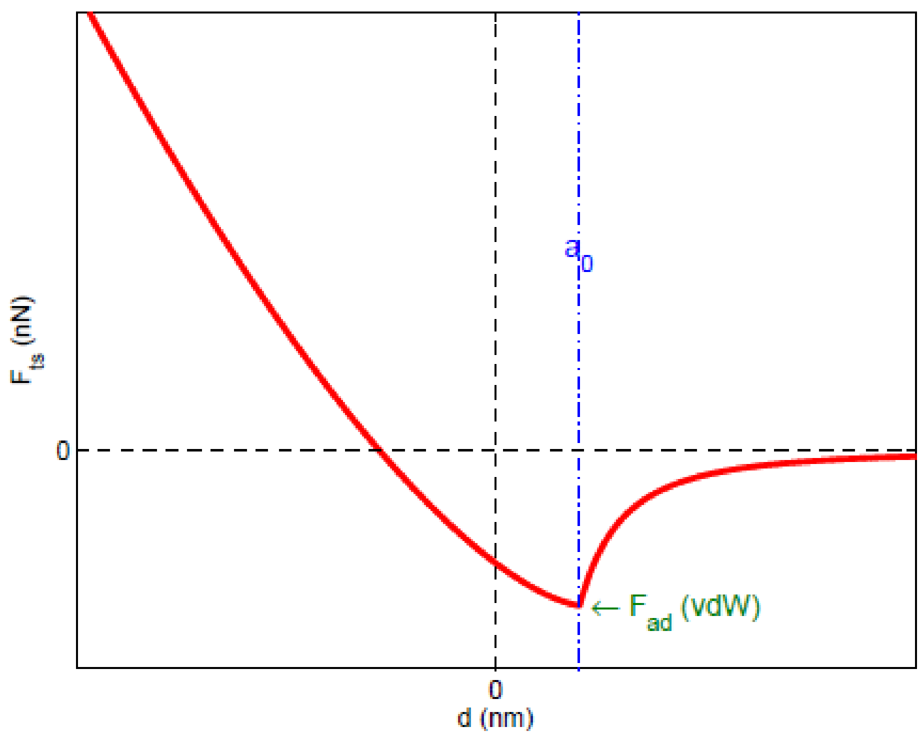
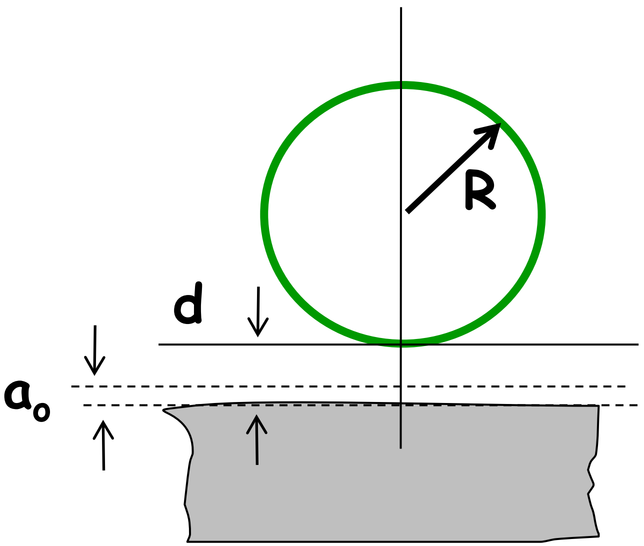
## DMT

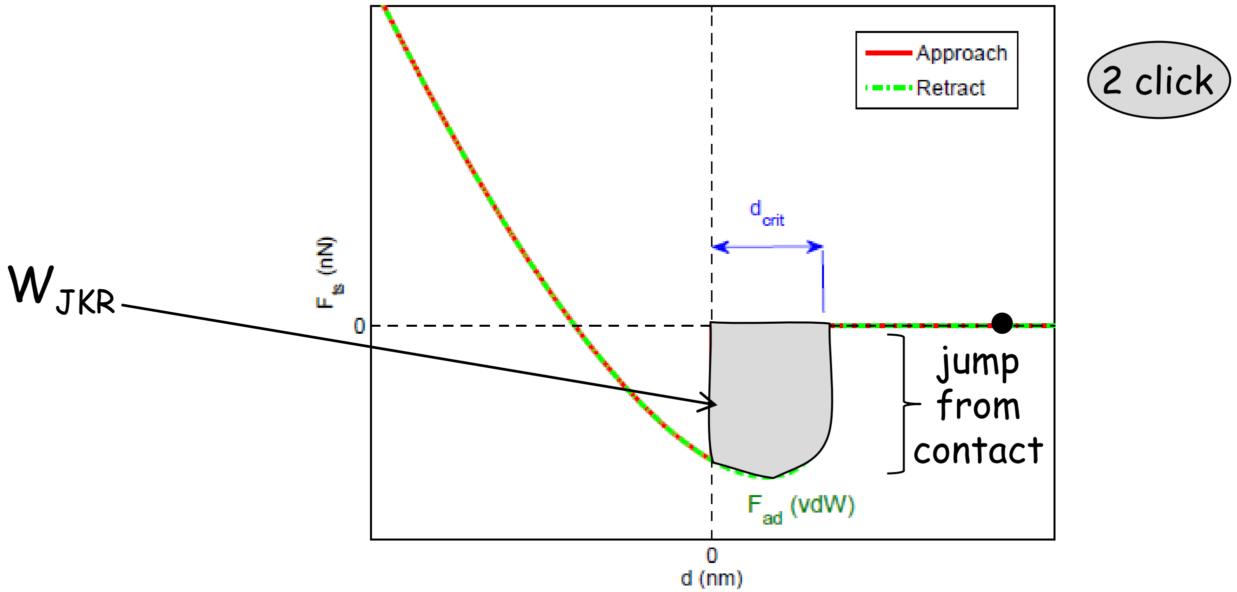



$$F_{ts}(d) = \begin{cases} -\dfrac{HR}{6d^2}, & d > a_o \\ -\dfrac{HR}{6a_o^2} + \dfrac{4}{3}E^*\sqrt{R}(a_o - d)^{3/2}, & d \le a_o \end{cases}$$

$$E^* = \left[\frac{1-\nu_{tip}^2}{E_{tip}} + \frac{1-\nu_{sample}^2}{E_{sample}}\right]^{-1}$$

# JKR




$$F_{ts}(d) = \begin{cases} 0, & \textit{no contact} \\ \dfrac{4E^* a^3}{3R} - \sqrt{8\pi W_{JKR} E^* a^3}, & \textit{contact} \end{cases}$$

$$W_{JKR} = \frac{2F_{adhesion}}{3\pi R}$$

$$d = -\frac{a^2}{R} + \sqrt{\frac{2\pi W_{JKR} a}{E^*}}$$

$$d_{critical} = \sqrt{\frac{2\pi W_{JKR} a}{E^*}} - \frac{a_{critical}^2}{R}; \quad a_{critical} = \left[\frac{\pi R^2 W_{JKR}}{8E^*}\right]^{1/3}$$

$$E^* = \left[\frac{1-\nu_{tip}^2}{E_{tip}} + \frac{1-\nu_{sample}^2}{E_{sample}}\right]^{-1}$$

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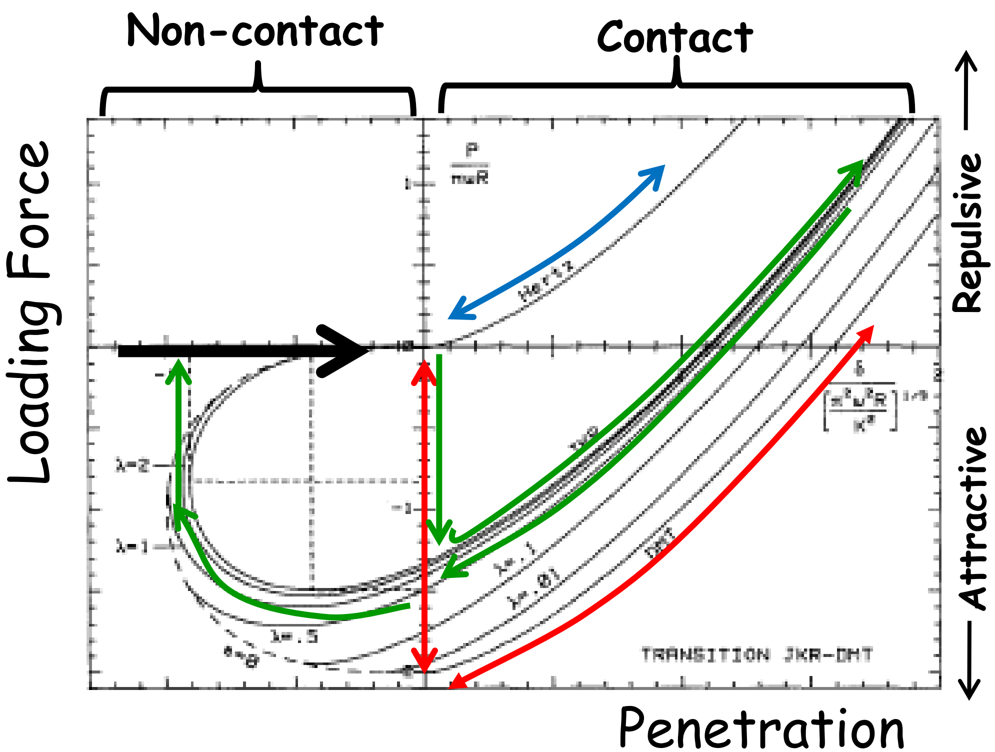
# Contact forces: Maugis' Theory

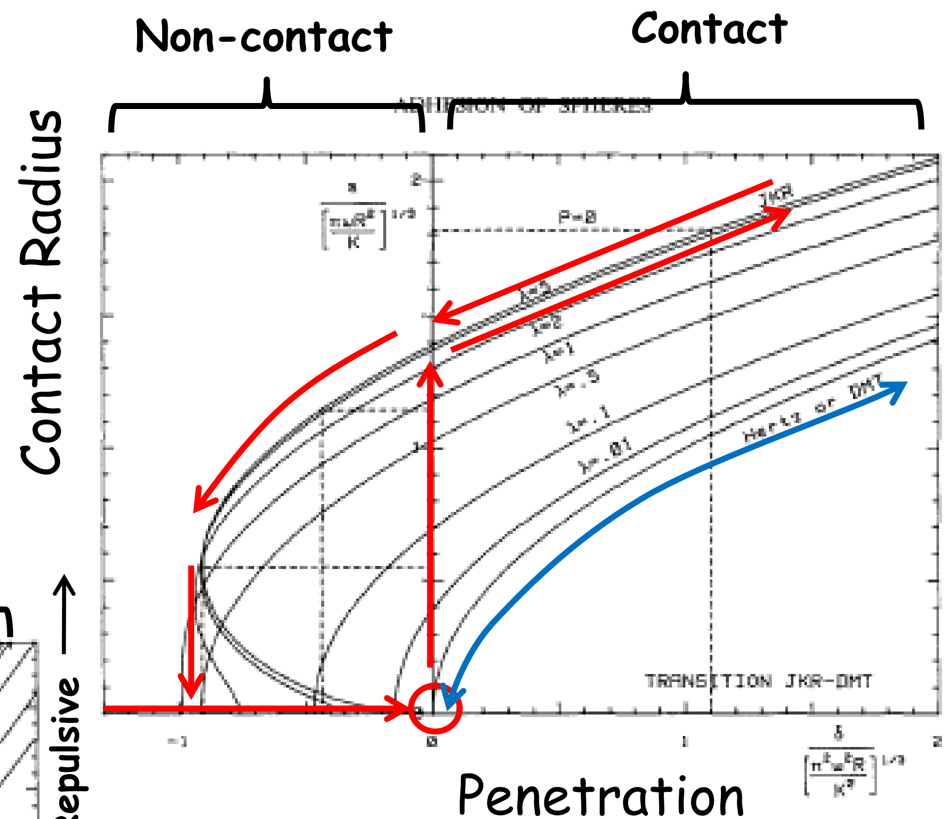
a: normalized contact radius
δ: normalized penetration
P: normalized force

$$\lambda = \frac{2.06}{a_0}\left(\frac{R_{tip}W_{132}}{\pi E_{tot}^{2}}\right)^{1/3} \propto \frac{adhesion}{elasticity}$$

$$\frac{1}{E_{tot}} = \frac{3}{4}\left(\frac{1-\nu_s^{2}}{E_s} + \frac{1-\nu_t^{2}}{E_t}\right)$$

$$a_o = r^* = \text{interatomic distance}$$

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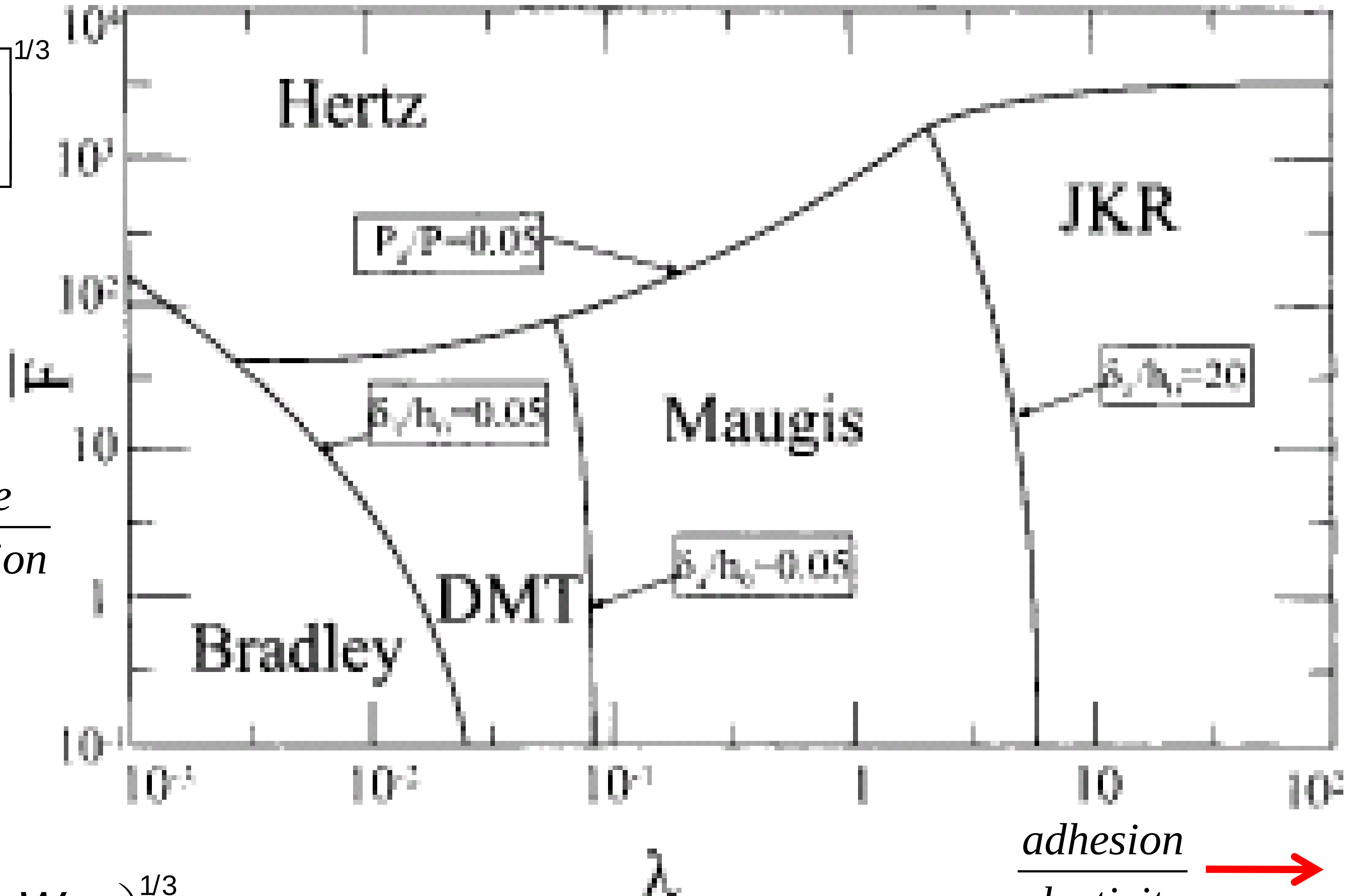
Λ→ 0: DMT (stiff materials)
Λ→ ∞: JKR (soft materials)

D. Maugis, J. Colloid Interface Sci.150, 243 (1992)

# Validity of different models – converting measured adhesion force to work of adhesion

$$\bar{F} = \left[ \frac{F}{\pi W_{132} R_{tip}} \right]^{1/3}$$

$$\frac{applied\ \ force}{work\ of\ \ adhesion}$$




$$\frac{adhesion}{elasticity}$$

$$\lambda = \frac{2.06}{a_0}\left( \frac{R_{tip} W_{132}}{\pi E_{tot}^{\ 2}} \right)^{1/3}$$

$$\frac{1}{E_{tot}} = \frac{3}{4}\left( \frac{1-\nu_s^{\ 2}}{E_s} + \frac{1-\nu_t^{\ 2}}{E_t} \right)$$

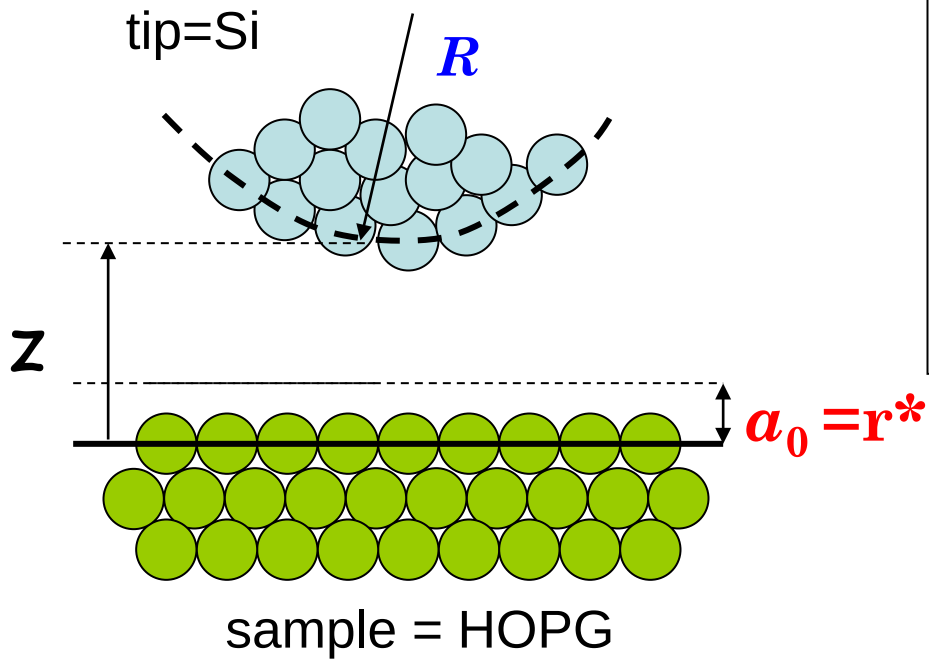
$a_0$ = equilibrium separation (typical atomic distance)

# Comments on these theories

- JKR predicts infinite stress at edge of contact circle.
- In the limit of small adhesion JKR -> DMT
- Most equations of JKR and Hertz and DMT have been tested experimentally on molecularly smooth surfaces and found to apply extremely well
- Most practical limitation for AFM is that no tip is a perfect smooth sphere, small asperities make a big difference.
- Hertz, DMT describe conservative interaction forces, but in JKR, the interaction itself is non-conservative (why?) …for a force to be considered conservative it has to be describable as a gradient of potential energy.

# Combining van der Waals force & DMT contact

$$F_i(z) = \begin{cases} -\dfrac{AR}{6z^2}, & (\text{for } z > a_0) \\ -\dfrac{AR}{6a_0^2} + \dfrac{4}{3}E^*\sqrt{R}\,(a_0 - z)^{3/2}, & (\text{for } z \le a_0) \end{cases}$$




$A$ : Hamaker constant (Si-HOPG)

$R$ : Tip radius

$E^*$ : Effective elastic modulus

$a_0$ : Intermolecular distance

*Raman et al, Phys Rev B (2002), Ultramicroscopy (2003)*