Lecture: P1_Wk2_L5

Contact Mechanics

Predict the stresses and deformations which arise when the surfaces of two solid bodies are brought into contact, subject to surface constraints.

Ron Reifenberger

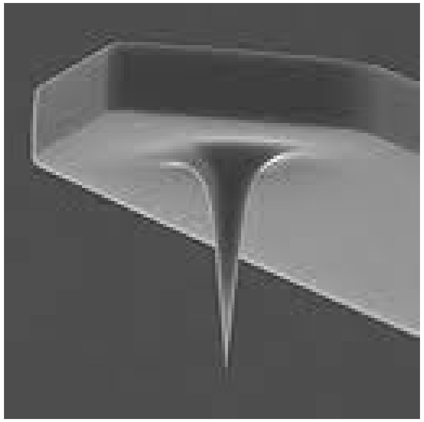
Birck Nanotechnology Center

Purdue University

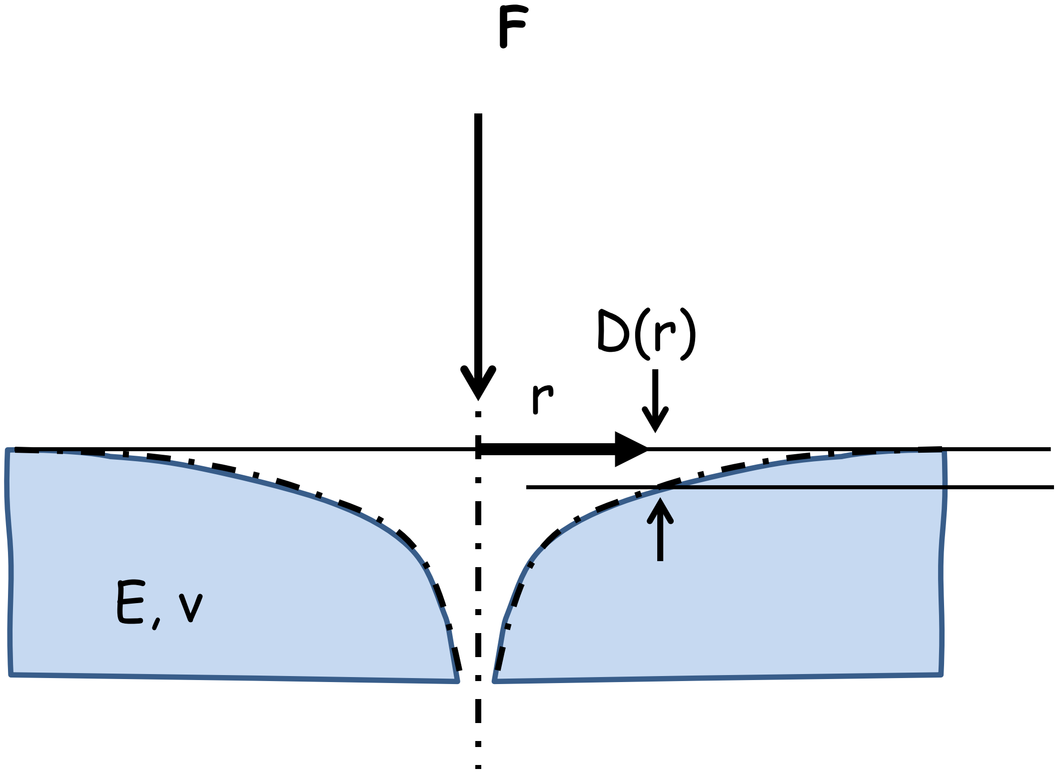
2012

PURDUE UNIVERSITY

Action of a point force (Boussinesq, 1885)



www. team-nanotec.de

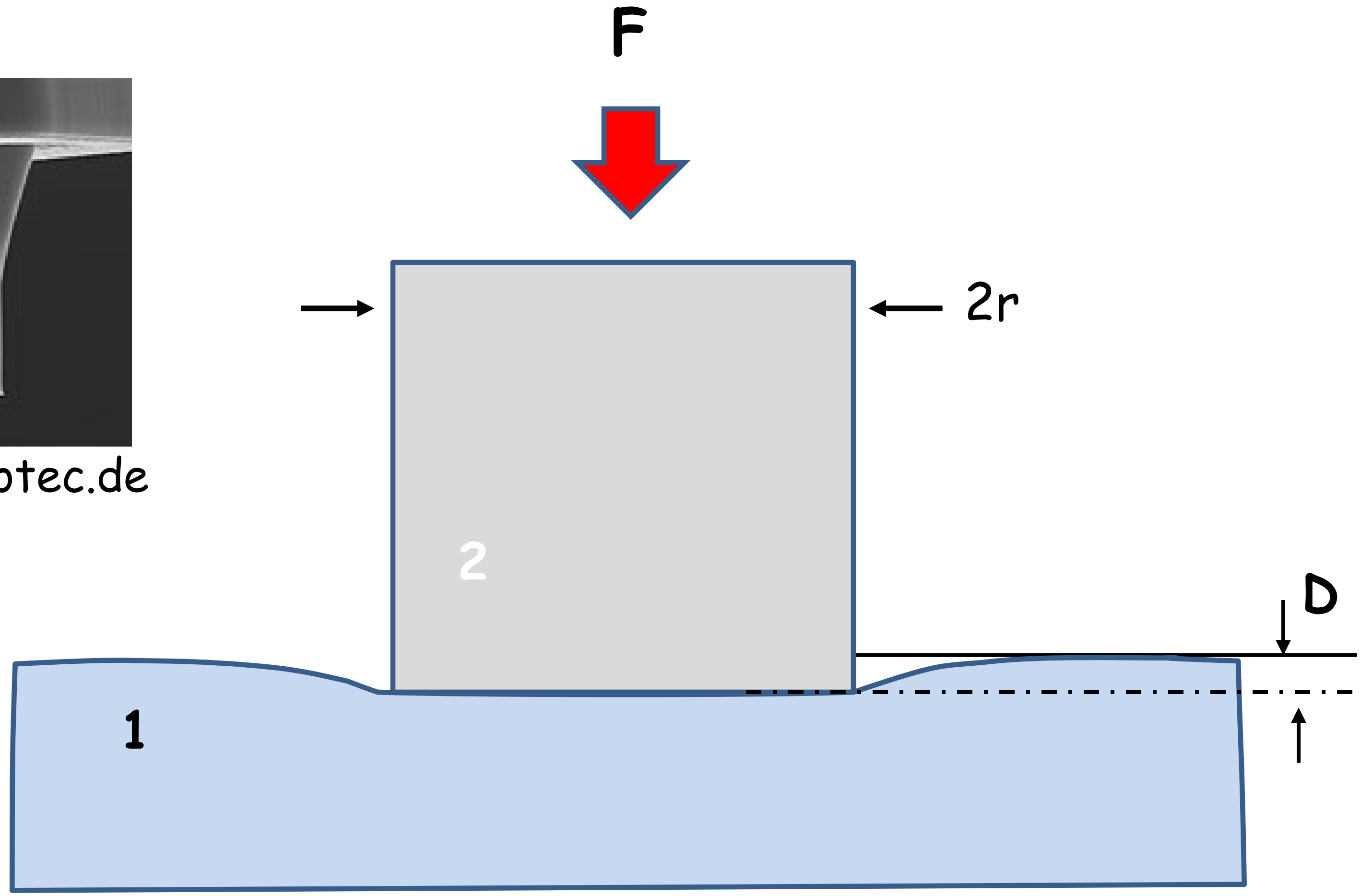


$$D(r) = \frac{1-\nu^2}{\pi E}\frac{F}{r}$$

Singular at r=0!

Action of a punch with circular cross-section

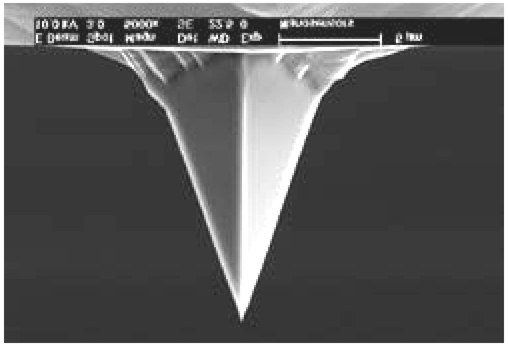
www. team-nanotec.de



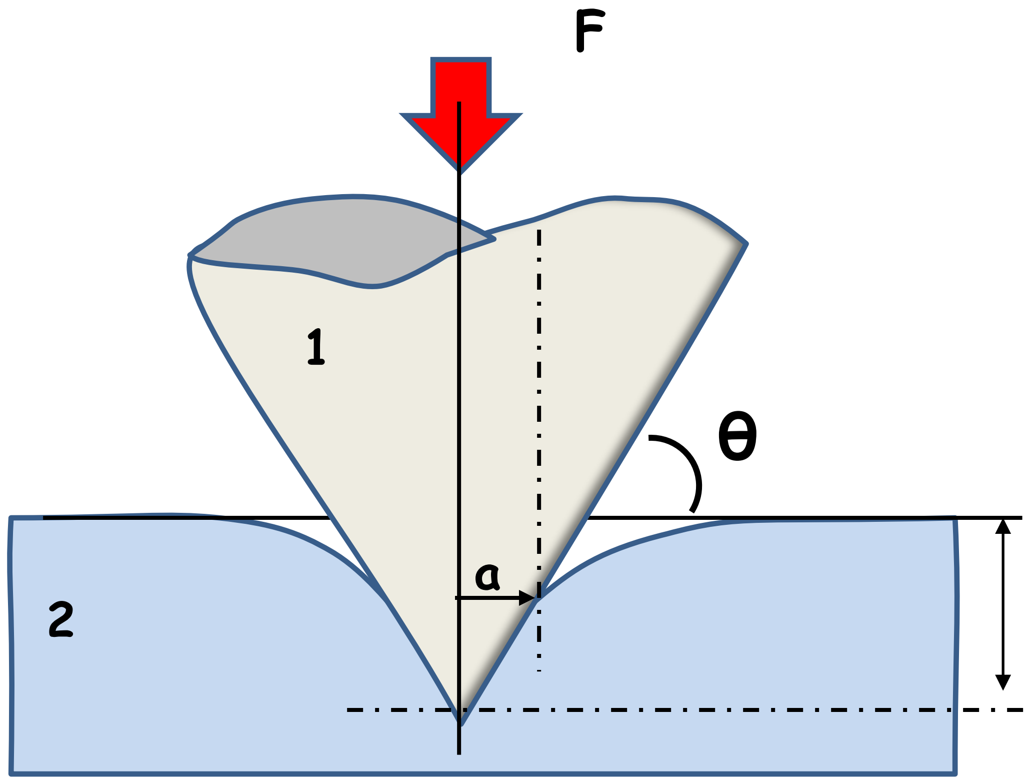
$$F = 2rE^{*}D$$

$$\left(\frac{1-\nu_1^{\,2}}{E_1} + \frac{1-\nu_2^{\,2}}{E_2}\right) = \frac{1}{E^{*}}$$

Action of a cone-shaped punch



http://www.nanosensors.com

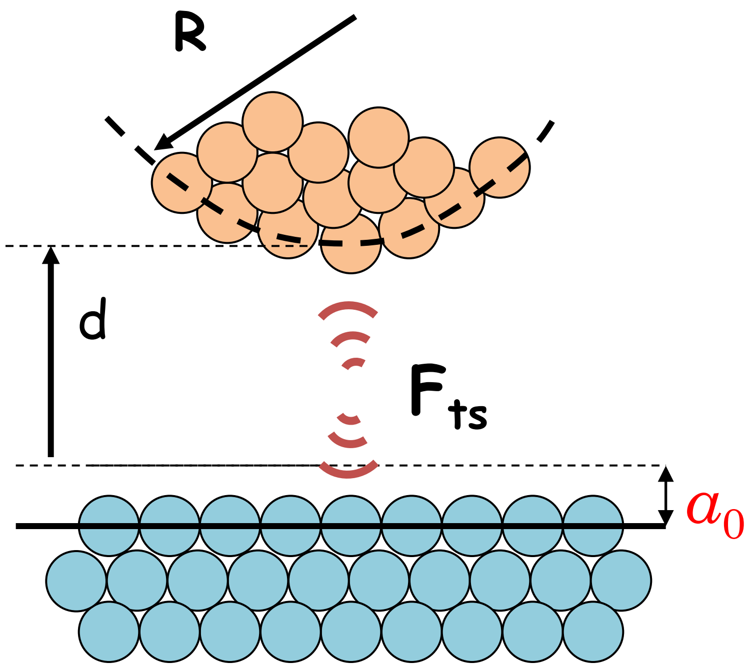


$$F = \frac{2}{\pi}\frac{E^*}{\tan\theta}D^2$$

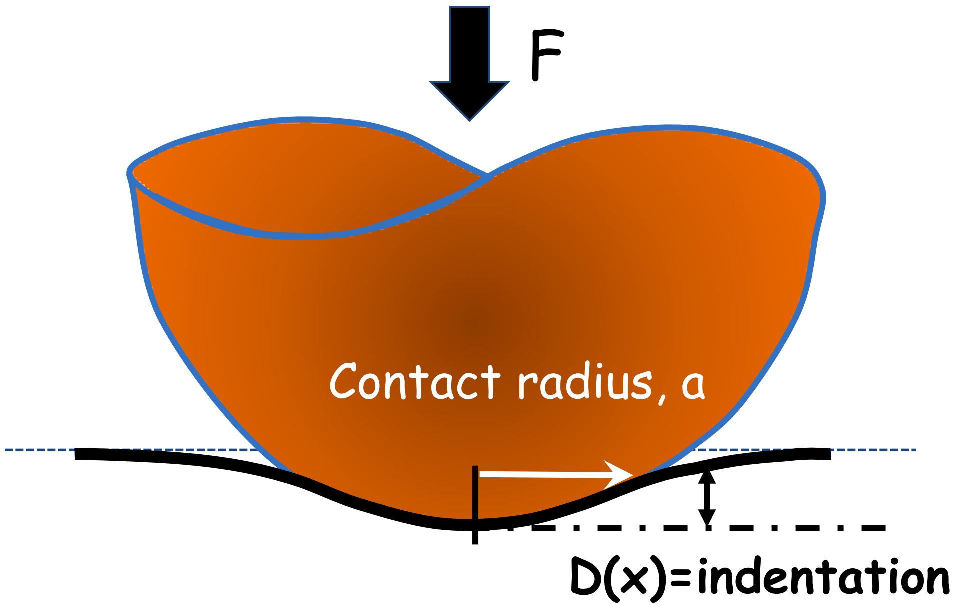
$$\left(\frac{1-\nu_1^{\,2}}{E_1}+\frac{1-\nu_2^{\,2}}{E_2}\right)=\frac{1}{E^*}$$

At a microscopic scale, for small indentations. . . .

AFM Problem

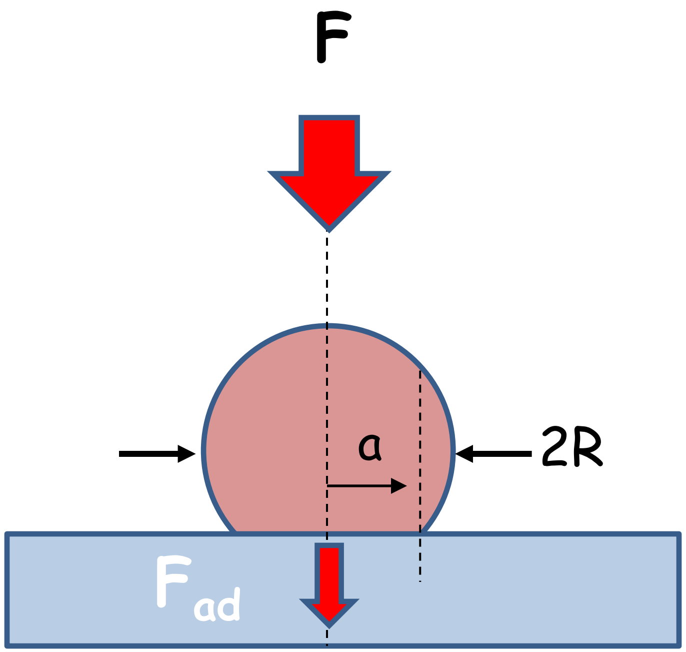


Contact Mechanics Literature



Use contact mechanics to make predictions for two quantities as a function of the applied force F

The basic problem



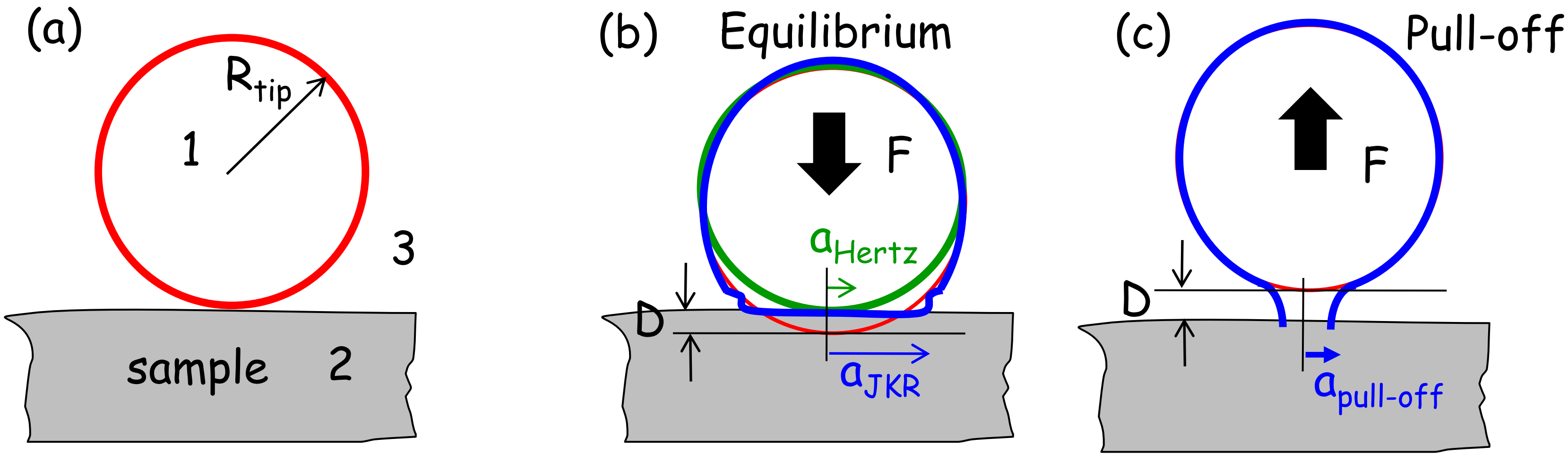
Quantities of interest:

- Contact radius (a)
- Adhesive Force (F_{ad})
- Contact radius at zero load (F=0)
- Contact radius at separation
- Pull-off force

Three Classic Theories

Hertz	Johnson-Kendall-Roberts **(JKR)**	Derjaguin-Muller-Toporov **(DMT)**

Need to Develop a Tip-sample Interaction Model



Rigid tip-**rigid** sample vs. **Deformable** tip and **rigid** sample*

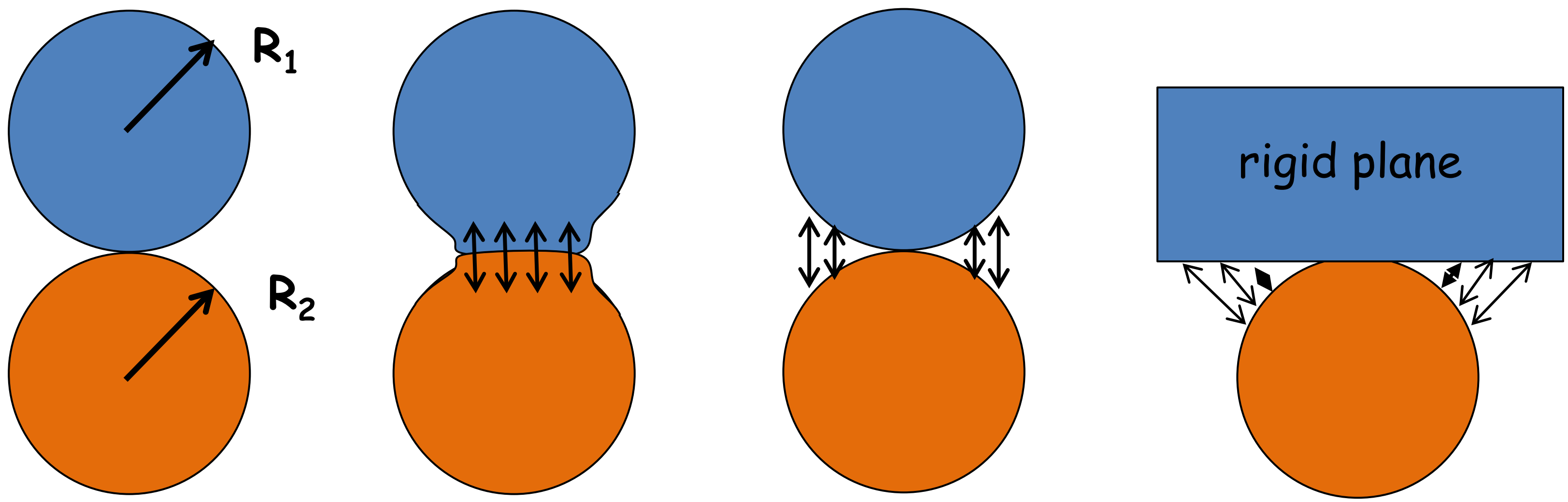
- From the Derjaguin approximation for rigid tip interacting with rigid sample (a) we have

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

- Real tips and samples are not rigid (see b,c above). Several theories have been developed to better account for this fact
- * Theories also apply to deformable samples; a rigid sample is shown only to demonstrate key quantities clearly. For example D is the combined tip-sample deformation in (b)

Classic Tip-Sample Interaction Models
(flat plane = $R_1 \rightarrow \infty$)

elastic	elastic, with adhesion in contact region	vdW with rigid spheres	elastic, adhesive and vdW



Hertz (1881)	JKR (1971)	Bradley (1932)	DMT 1975
•Neglects surface forces and adhesion •Assumes a linearly elastic sphere indenting an elastic surface	•Neglects long-range interactions outside contact area •Applicable to soft samples with high adhesion	•Considers two rigid spheres interacting *via* Lennard-Jones 6-12 potential	•Elastic sphere against a rigid plane surface • Includes van der Waals forces outside the contact region. •Applicable to stiff samples with low adhesion.

K.L. Johnson, *Contact Mechanics* (Cambridge University Press, 1985)

Surface forces give rise to surface energies

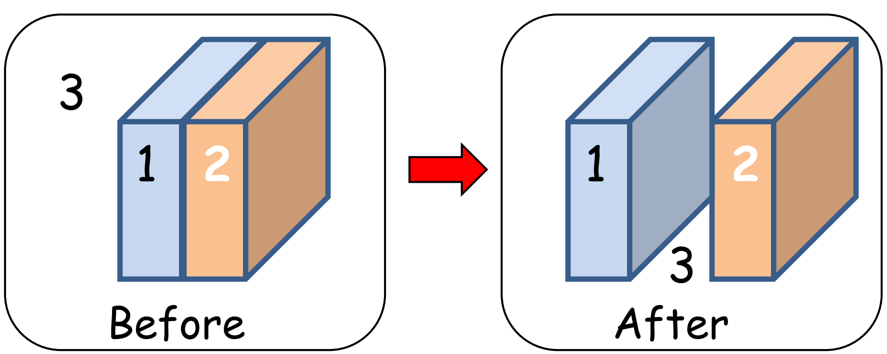
- Work of adhesion and cohesion: work done to separate unit areas of two materials 1 and 2 from contact to infinity in vacuum. If 1 and 2 are different then W_{12} is the work of **adhesion**; if 1 and 2 are the same then W_{11} is the work of **cohesion**.
- Surface energy: This is the free energy change when the surface area of a material is increased by unit area:

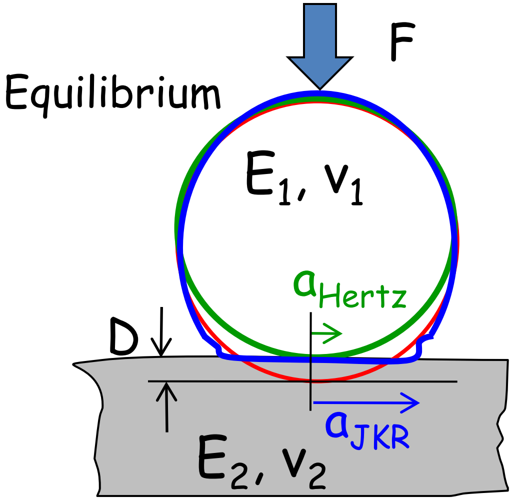
$$W_{11}\left(=\gamma_{11}\right)=2\gamma_1 \quad \left[{}^{J}\!/_{m^2}\right]$$

(see lecture P1_Wk2_L2)

- When separating dissimilar materials, the free energy change in destroying the existing "interfacial" area per unit area is known as the interfacial energy γ_{12}
- Work of adhesion in a third medium: *in a vacuum*, $W_{12}=\gamma_1+\gamma_2-\gamma_{12}$

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





Standard results

$$\frac{1}{E_{tot}} = \frac{3}{4}\left(\frac{1-\nu_1^{\,2}}{E_1} + \frac{1-\nu_2^{\,2}}{E_2}\right) = \frac{3}{4}\frac{1}{E^*}$$

"*springs in series*"

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

	$F_{pull\text{-}off} = F_{ad}$ (a)	Contact Radius (b,c)	Deformation(c)
Hertz	0	$a_{Hertz} = \left(\frac{R_{tip}F}{E_{tot}}\right)^{1/3}$	$D_{Hertz} = \frac{a_{Hertz}^2}{R_{tip}}$
DMT	$F_{ad}^{DMT} = 2\pi R_{tip} W_{132}$	$a_{DMT} = \left(\frac{R_{tip}\left[F + F_{ad}^{DMT}\right]}{E_{tot}}\right)^{1/3}$	$D_{DMT} = \frac{a_{DMT}^2}{R_{tip}}$
JKR	$F_{ad}^{JKR} = \frac{3\pi}{2} R_{tip} W_{132}$	$a_{JKR} = \left(\frac{R_{tip}}{E_{tot}}\left[\sqrt{F_{ad}^{JKR}} + \sqrt{F + F_{ad}^{JKR}}\right]^2\right)^{1/3}$	$D_{JKR} = \frac{a_{JKR}^2}{R_{tip}} - \frac{4}{3}\sqrt{\frac{F_{ad}^{JKR}\,a_{JKR}}{R_{tip}\,E_{tot}}}$

Notes:

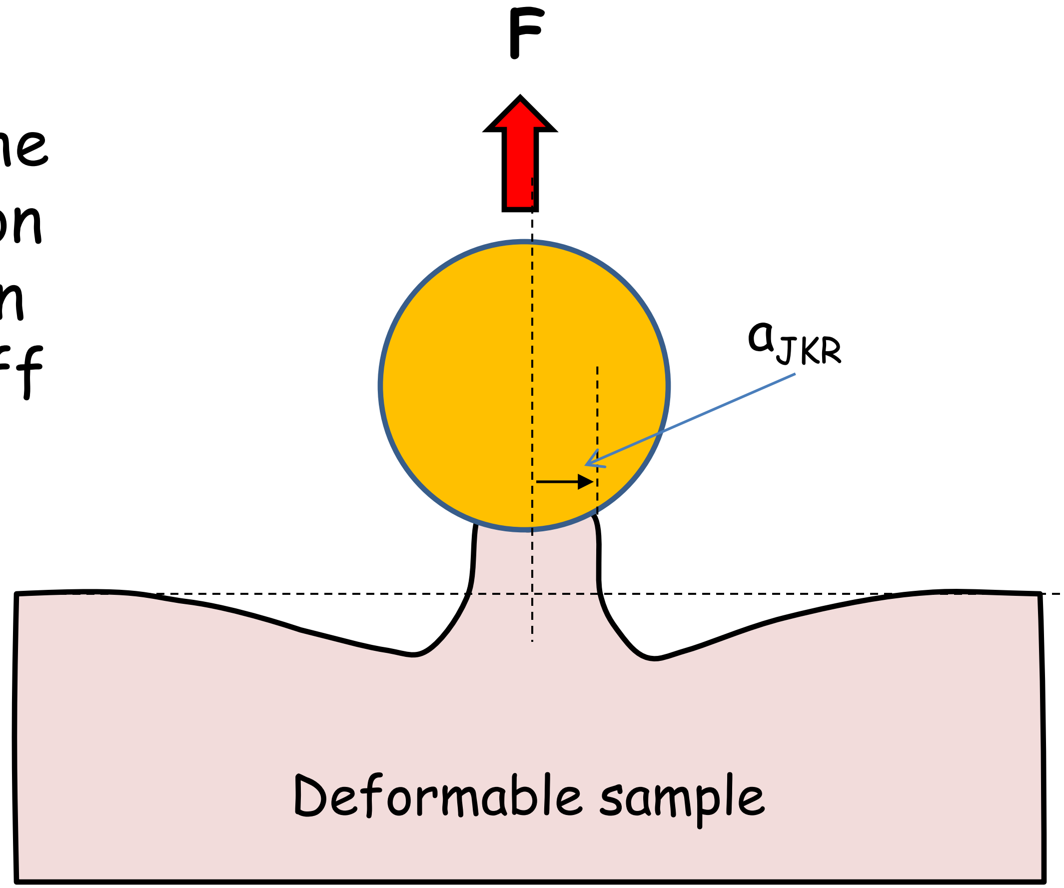
(a) No surface forces → $W_{132}=0$

(b) Hard to define accurately when contacts are small

(c) Adhesive correction

JKR Adhesion - consequences

Adhesion arises fundamentally from the short range interaction between molecules. In the JKR model, pull-off occurs when contact radius a_{JKR}=0



Warning - major limitation of classical results: Surface roughness

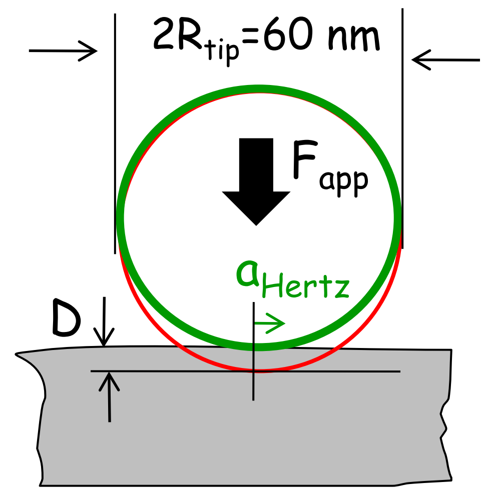
Example

<u>Hertz contact</u>: 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:

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

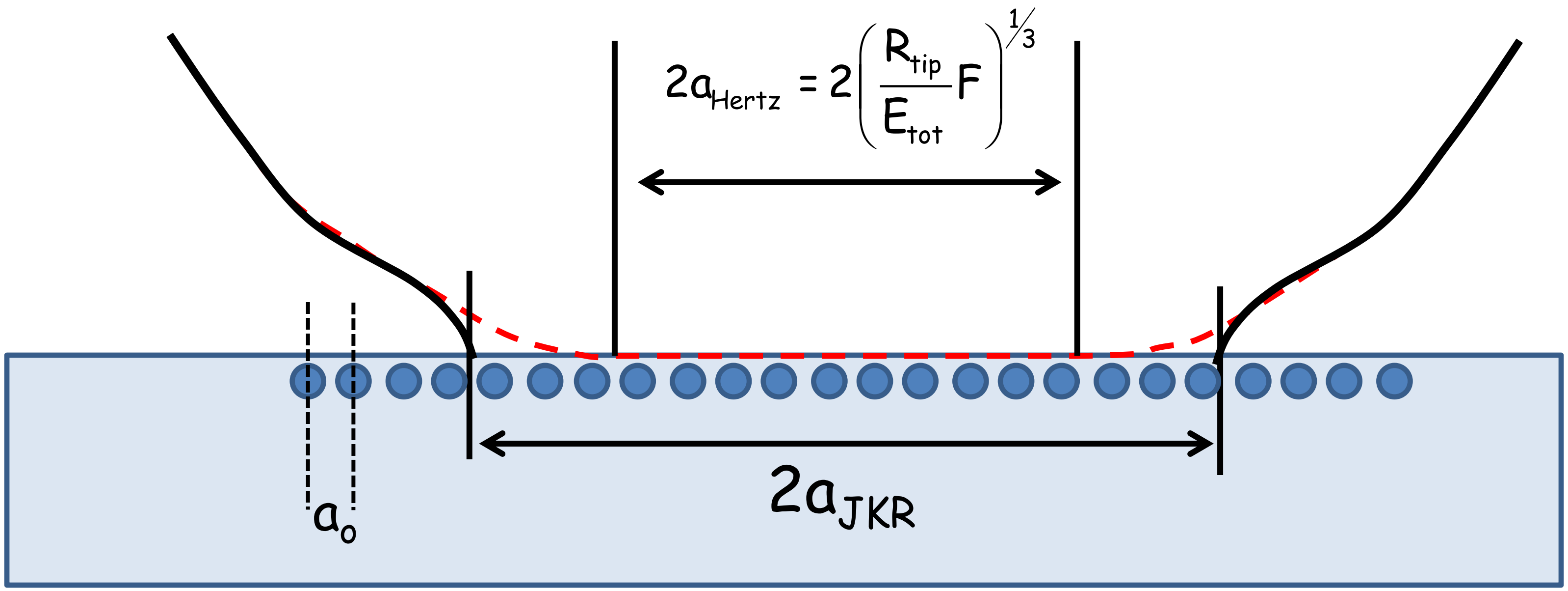
Deformation:

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

Pull-off Force=0

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

Which contact model to choose?

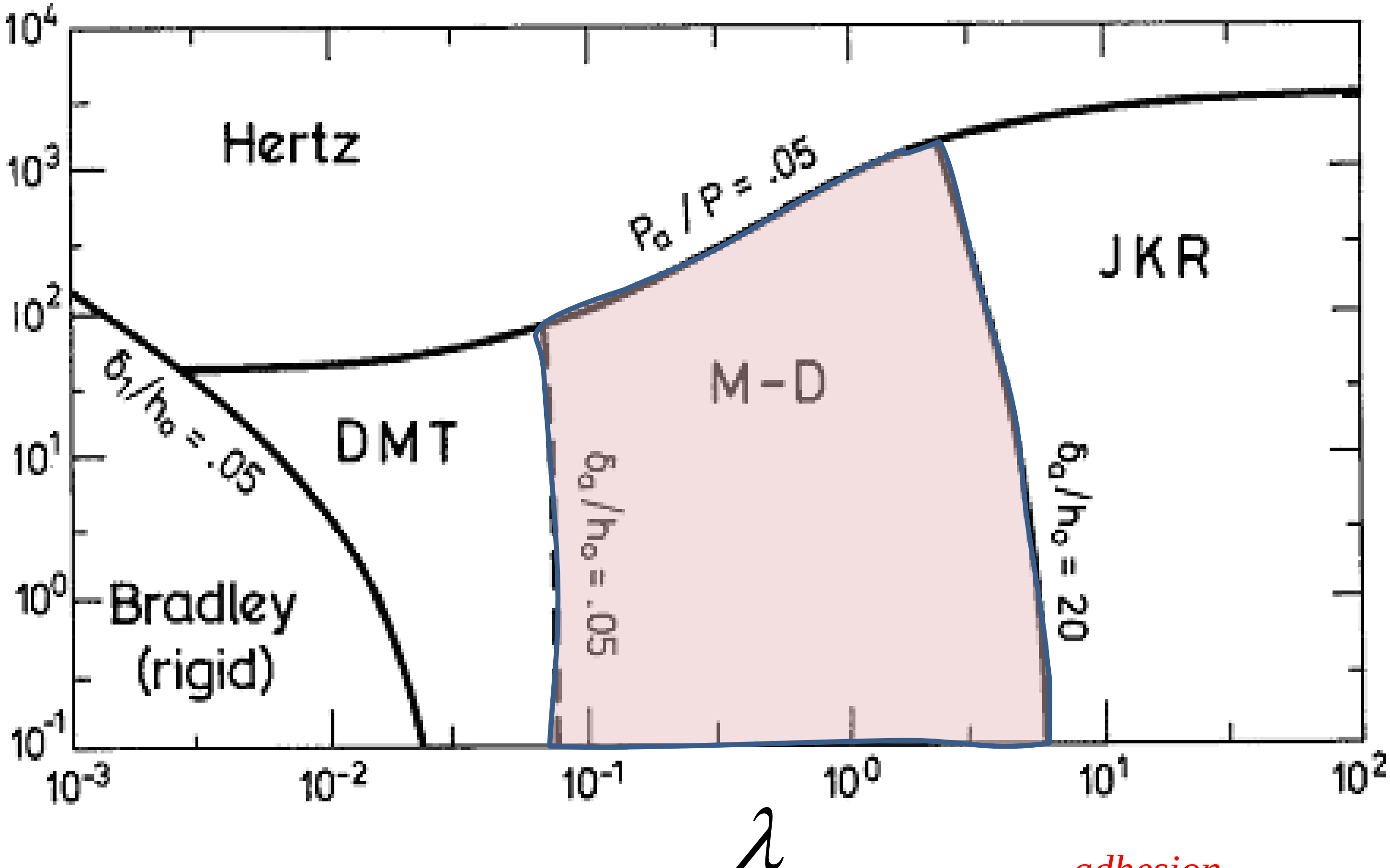


$$\text{define new parameter} \propto \frac{\text{width of elastically deformed neck}}{\text{atomic spacing}}$$

$$\mu = \frac{\frac{32}{3\pi}\left(\frac{2R_{tip}W_{132}^2}{\pi E_{tot}^2}\right)^{1/3}}{a_0} = 4.27\frac{\left(\frac{R_{tip}}{E_{tot}}\cdot\frac{W_{132}^2}{\pi E_{tot}}\right)^{1/3}}{a_0} \quad [\text{no dimensions}]$$

$$\lambda = \frac{2}{a_0}\left(\frac{9R_{tip}W_{132}^2}{16\pi E_{tot}^2}\right)^{1/3} = \frac{2}{a_0}\left(\frac{9}{16}\right)^{1/3}\left(\frac{R_{tip}W_{132}^2}{\pi E_{tot}^2}\right)^{1/3} = 1.65\frac{\left(\frac{R_{tip}}{E_{tot}}\cdot\frac{W_{132}^2}{\pi E_{tot}}\right)^{1/3}}{a_0} \quad [\text{no dimensions}]$$

Validity of different models



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

$$\propto \frac{applied\ \ force}{adhesion}$$

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

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

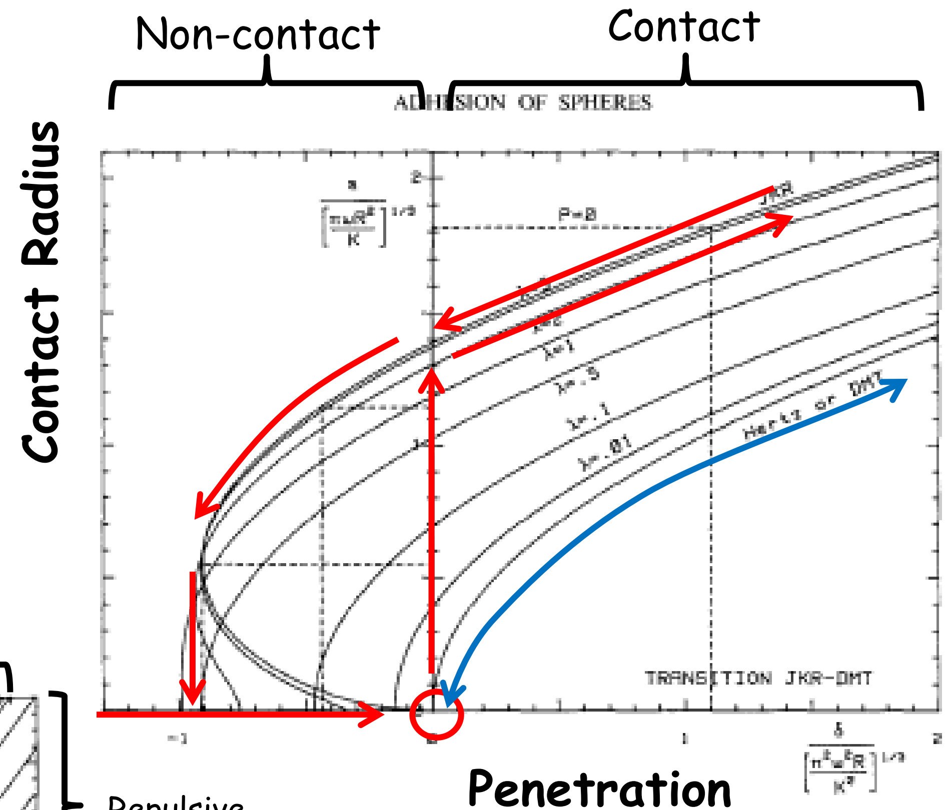
$$a_0 = (typical\ atomic\ spacing)$$

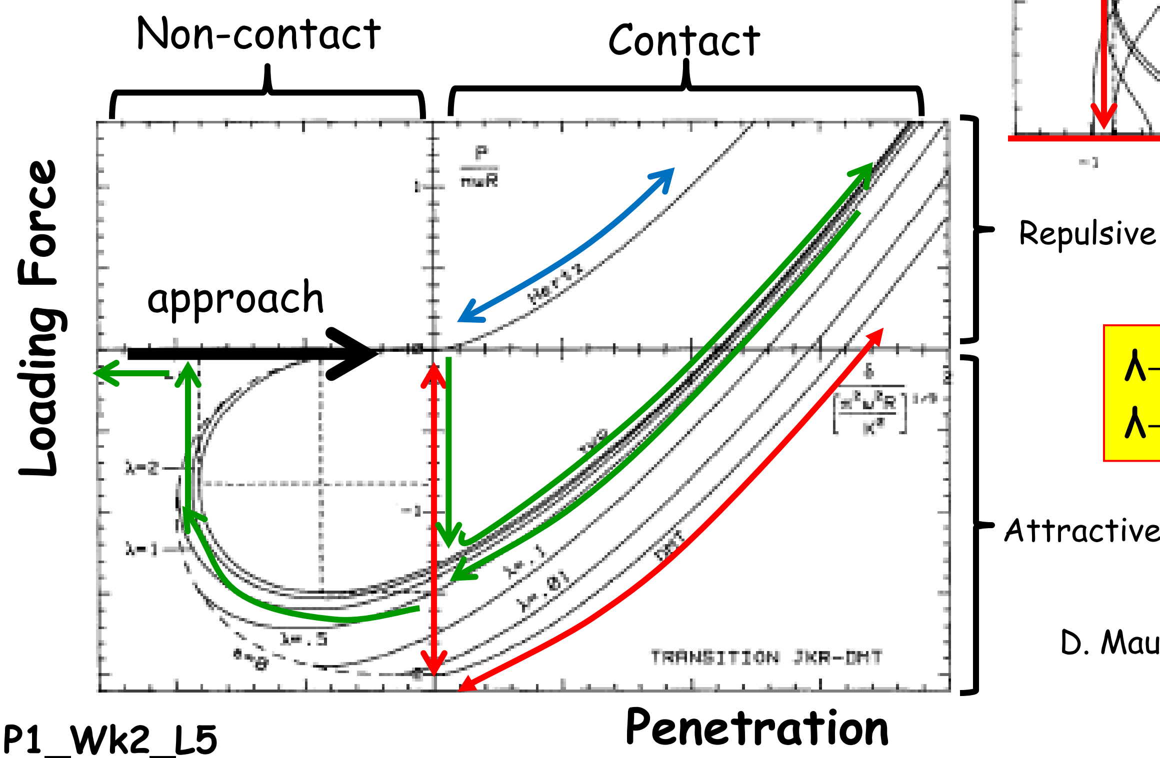
Transition from DMT to JKR: Maugis-Dugdale Theory

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

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

$$a_o = \text{interatomic distance}$$





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

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

Up Next: Combining contact mechanics with intermolecular interactions

Appendix: A few comments on these theories

- 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
- The limitation for application to AFM is that no tip is a perfectly 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 must be written as a gradient of potential energy.