A Short Course on Nanoscale Mechanical Characterization: The Theory and Practice of Contact Probe Techniques

Tuesday, Part 1: Contact Mechanics

- Hertz & Boussinesq Problem
- Adhesive elastic contact mechanics
- Fracture approaches to the adhesive problem
- Elastic-plastic problem
- Viscoelastic problem
- Rough surfaces

Hertz & Boussinesq Problem
Hertz Theory of Contact

- Assumptions:
  - contacting bodies are HILE
  - contact radius is small compared to the size & curvature radius of the bodies
  - frictionless surfaces

- Contact pressure, contact size, surface compression all depend on the load in a non-linear manner

- Consider two spheres in contact, radii \( d_1/2 = R_1, d_2/2 = R_2 \); moduli \( E_1, E_2 \); Poisson’s ratios \( \nu_1, \nu_2 \). Applied load = \( P \)

**Hertz Equations**

Define: \( R_{\text{off}} = \left( \frac{1}{2} R_1 + \frac{1}{2} R_2 \right) \), \( E^* = \left( \frac{1}{2} E_1 + \frac{1}{2} E_2 \right) \)

- Contact radius: 
- Surface compression: \( C = C_1 + C_2 = \)
- Max. normal pressure at interface: \( p_0 = \frac{3}{2} P_{\text{ave}} = \)

where \( P_{\text{ave}} = P/R^2 \)

- Normal stress: \( C_z(r) = \)

at the contact zone edge:

\( C = 0.13 p_0, C_1 = 0.13 p_0, C_z = 0 \)

which is a state of pure shear!
Hertz Theory of Contact

- An analytic solution for all stress components at all points in space exists.
- Note: the largest shear stress $t_{\text{max}} = 0.31p_0$ occurs at...
- The theory can also be applied to a sphere contacting a flat plane by letting...
- Exercise: simplify the Hertz equations for this case, assuming the materials are the same.

Boussinesq Problem: Rigid flat punch

- The stress distribution is very different for a rigid circular punch:
  
  \[ a = \text{constant} \]
  
  surface compression: $\square$
  
  max. normal pressure: $p_0 = \frac{1}{2}p_{\text{ave}}$
  
  normal stress: $s_z(r) = \square$
Uniform pressure vs. Hertz pressure

- Uniform pressure: stress is directly proportional to load, contact area is constant.
- Hertz pressure: stress depends nonlinearly on load, contact area is changing with load.

**Design considerations:** bearing life is strongly influenced by contact stresses. For example, for ball bearings, fatigue life is related to $p_0^{-9}$. Thus, small reductions in stress can substantially affect bearing performance.

Adhesive elastic problem
Recall: The JKR theory predicts the effect of adhesion on the contact area

\[ A = \pi a^2 \]

\[ A = \frac{3R^3}{E^*L} + \frac{3\gamma}{R} + \frac{6\gamma}{R} + \frac{3\gamma}{R} \left( \frac{1}{3} \right) \]

\[ \gamma = \text{interfacial energy} \]

**Hertz:** 
\[ A = \frac{3R^3}{E^*L} \]

**JKR:** 
\[ A = \frac{3R^3}{E^*L} + \frac{3\gamma}{R} + \frac{6\gamma}{R} + \frac{3\gamma}{R} \left( \frac{1}{3} \right) \]

The area of contact depends upon the range of the attractive forces

**\( D < 0.1 \) (DMT)**

**\( D > 5 \) (JKR)**

Johnson-Kendall-Roberts (JKR): short-range forces, high adhesion, compliant materials

Derjaguin-Müller-Toporov (DMT): long-range forces, low adhesion, stiff materials

Intermediate cases: Maugis, Colloid Interface Sci. 1992, 150, 243.
Recall: Ac depends on the range of the attractive forces

DMT=Derjaguin-Müller-Toporov model
Derjaguin, B. V.; Muller, V. M.; Toporov, Y. P. J. Colloid Interface Sci. 1975, 53, 314.
Recall: How to tell if you are in the JKR or DMT regime (or in between)?

- compare the elastic deformation that adhesion forces cause with the range of the adhesion forces themselves

\[ f = \frac{1}{3} \sqrt{\frac{g^2}{R^2 E^* z_0^3}} \]

- \( f \) = adhesion energy
- \( R \) = tip radius
- \( E^* \) = elastic modulus
- \( z_0 \) = equilibrium spacing

Fracture mechanics approaches to adhesive contact and friction
Contact -- Crack

- Tip/sample contact is analogous to an external circular crack
- System is otherwise elastic

JKR Theory of Contacts

- Griffith’s concept of brittle fracture
- Total load: \( P = P_{\text{Hertz}} + (\Box P_a) \), \( P_{\text{Hertz}} = \frac{4}{3} E^* \cdot \frac{a^3}{R} \)
- Mode I stress intensity factor \( K_I \), Irwin’s relationship:
  \[
  K_I = \frac{1}{2} \sqrt{\frac{2a}{P_a} \cdot \sqrt{2a}} = \frac{P_a}{2a \sqrt{P_a}} \quad G = \frac{K_I^2}{2E^*} = \square
  \]
- Final result:
  \[
  a^3 = \frac{R}{4E^*} P + \frac{3}{4} R P + \left( \frac{3}{4} R P \right)^2 + \left( \frac{3}{4} R P \right)^2
  \]
  \( a = \) contact radius \( P = \) load \( R = \) tip radius \( g = \) adhesion energy \( E^* = \) reduced Young’s modulus
Maugis’ Dugdale Model

Assumptions of Maugis’ model

1. Linear elastic fracture mechanics applies
2. Link between equilibrium spacing and cohesive zone distance:

\[ \delta_0 = \delta_{\text{theoretical, LJ}} \]
\[ \delta_{\text{theoretical, LJ}} = 1.03 \frac{\gamma}{\sigma_0} \]
\[ G = \frac{\delta_0 \cdot \delta}{\delta_0}, ~ G = \frac{\delta_0 \cdot \delta}{\delta_0} = 1.03 \cdot \delta \]

Shear strength measurements using the MD model are now being made by several groups

- Lantz et al. (Phys. Rev. B 1997, 55, 10776): Si/NbSe₂
- Pietrement & Troyon (Langmuir 2001, 17, 6540): SiNₓ/carbon fiber, SiNₓ/mica, SiNₓ/SiO, SiNₓ/epoxy
- Observations include: load-dependent shear strengths in some cases, more near-ideal shear strengths, correlation between friction and adhesion
- E. Barthel (J. Colloid Interface Sci. 1998, 200, 7), has shown that the details of the interfacial potential do not strongly affect the contact behavior
Kim & Hurtado’s model


- why is the shear strength so large for AFM results, but typically much smaller for larger?
- use a dislocation mechanics approach
- predicts a scale dependence of shear strength
Kim & Hurtado’s model

Elastic-plastic problem
Elastic-plastic indentation

from Johnson, Contact Mechanics

Contact of Rough Surfaces
Mechanics Issues in MEMS: Friction and wear

• Currently, there are no commercial MEMS devices that involve contacting surfaces with extended sliding

![AFM images of polycrystalline MEMS surface](image)

AFM images of polycrystalline MEMS surface
(E. Flater & R. Carpick)

- 10 x 10 µm scan, 100 nm scale
- RMS roughness ~11.5 nm
- 500 x 500 nm scan, 30 nm height scale
A multi-scale understanding of friction could be developed through experiment and modeling:

- Prediction, design, understanding
- Micromachine interface
- Mechanics of multi-asperity contacts
- Topographic studies; constitutive laws for friction & wear
- Single asperity: $F_f = \mu P A$ (?)
- Multiple asperities: $F_f = \mu L (?)$

Contact mechanics analysis: the Greenwood-Williamson Theory

- Distribution of summit heights
- Distribution of surface heights
- Rigid plane, lowered
- Rough elastic surface

GW Theory: Assumptions

- linear, elastic, homogeneous, isotropic
- distribution of peak heights is Gaussian
- radius of peaks is constant (or narrowly distributed about a mean)
- Hertzian contact (no adhesion, no tangential stresses)
- key parameters:
  - number of peaks/area
  - peak curvature
  - std. dev. of peak height distribution
  - elastic modulus

The GW Theory: Derivation

The GW Theory


\[ A_i = R(z_i - d) \quad L_i = KR^{1/2} (z_i - d)^{3/2} \]

Let \( R(z) \) = asperity height distribution

\[ \text{i.e. there are } N \text{ asperities between } z \text{ and } z + dz \]

total contact area \( A = \sum A_i \)

total load \( L = \sum L_i \)

Assume Gaussian distr. of summit heights: \( R(z) = \frac{1}{\sigma \sqrt{2\pi}} e^{-z^2/2\sigma^2} \)

then \( \frac{A}{L} = \int R(z) dz \)
The effect of increasing the load is

Note: real contact area may only be a fraction of a percent of the apparent contact area!

An explanation for macroscopic friction?

\[
\frac{A}{L} = \frac{\int R^{1/2}}{K^{1/2}} \cdot \int (x-a) e^{\frac{x^2}{2}} \, dx = \frac{\int R^{1/2}}{K^{1/2}} \cdot I
\]

\[
F_f = \int (x-a) e^{\frac{x^2}{2}} \, dx = \int R^{1/2} \cdot I
\]
Mistakes in the analysis

• How to correct for this?
• The answer comes from oceanography!
  – developed by Longuet-Higgins, *Phil. Trans. R. Soc. Lond.* (1957)
  – adapted to contact problems by Nayak, *J. Lubr. Technol.* (1971)
  – see work by J. I. McCool

Rough surfaces with adhesion

• Fuller & Tabor: JKR case
  • *The effect of surface roughness on the adhesion of elastic solids*
    • Proceedings of the Royal Society of London A. 1975; 345(1642): 327-42

• Maugis: DMT case
  • *On the contact and adhesion of rough surfaces*
    • Journal of Adhesion Science and Technology. 1996; 10(2): 161-75
Scale Effects in Plasticity

Hall-Petch Effect

Yield stress increases with decreasing grain size

\[ \sigma = \sigma_0 + kd^{-1/2} \]

\( d \) = grain size

Hardness of molybdenum thin films

Yoder et al, 2003

Indentation Size Effect & Reverse Indentation Size Effect

Ma and Clark J Mater. Res. 10(4)

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Indentation Size Effect & Reverse

Indentation Size Effect

FIG. 3. Hardness H versus plastic depth \( x_p \) for nanolamite and multilayer Cu/Nb thin films.

Tambwe et al, J Mat. Res. 1999
Surfaces

- Surface crystallography
- Relaxation and reconstruction
- Surface states
- Surface energy
- Characterization methods

Surface crystallography

- A 2-D lattice is referred to as a net
- The area unit is referred to as a mesh
- 5 Bravais nets in 2-D
  - Square
  - Hexagonal
  - Rectangular
  - Centered rectangular
  - Oblique
  - Mesh defined by mesh basis vectors $c_1, c_2$
  - For a reconstructed surface, $(c_1, c_2) \neq (a_1, a_2)$
Wood’s notation:
- used for reconstructed surfaces or overlayer (adsorbate) structures

- General relation between $c$’s and $a$’s:

$$[c_1, c_2] = P_{11} [a_1, a_2] = P_{12} [a_1, a_2] = P_{21} [a_1, a_2] = P_{22} [a_1, a_2]$$

- Wood’s notation:
  - $[]$ omitted if it is $0°$.
  - $p$ or $c$ is included at the beginning to indicate primitive or centered, e.g. $c(4x2)$, $p(2x2)$
    - The $p$ is optional
  - The surface is listed first, e.g. Si(111) (7x7)
  - If an adsorbate structure is being described, it is included afterward, e.g. Si(111) (1x1)H

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**Figure 9**

- (a) Square lattice: $|a_1| = |a_2|$, $\phi = 90°$
- (b) Hexagonal lattice: $|a_1| = |a_2|$, $\phi = 120°$
- (c) Rectangular lattice: $|a_1| = |a_2|$, $\phi = 90°$
- (d) Centered rectangular lattice: axes are shown for both the primitive cell and for the rectangular unit cell, for which $|a_1| = |a_2|$, $\phi = 90°$. 

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Examples:
- See: http://www.chem.qmw.ac.uk/surfaces/scc/ (Prof. R. Nix, U. London)

Substrate: fcc(100)
- c(2 x 2)
- (√2 x √2)R45

Substrate: fcc(110)
- c(2 x 2)

Substrate: fcc(111)
- (√3 x √3)R30

Surface Relaxation and Reconstruction
- Surfaces are defects: bonds are broken (all of them!), creating dangling bonds
- Atoms will re-arrange to make up for this lack of coordination
- Surface relaxations: motion of atoms inward or outward from surface plane
  - See table
  - Compensation for “electron overspill” (sketch)
- Surface reconstruction: rebonding of surface and sub-surface atoms
  - Surface lattice is
  - More frequently observed with
  - Can be removed by
  - e.g. Diamond(111)
Surface relaxations

Relaxation

- Relaxation: motion perpendicular to surface
  - change in the interlayer spacing.
  - Usually affects the first 1-3 layers, with the strongest effect at the surface.

Table 1  Relaxation of topmost interlayer spacing at unreconstructed clean metal surfaces

<table>
<thead>
<tr>
<th>Lattice</th>
<th>Relaxation</th>
<th>Material</th>
<th>Material</th>
<th>Material</th>
</tr>
</thead>
<tbody>
<tr>
<td>hcp(0001)</td>
<td>Re (+5%), Sc (+2%), Ti (+2%), Zr (+1%)</td>
<td>Al (+1%), Ag (0%), Cu (+0.7%), Pt (+1%), Rh (0%)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>fcc(111)</td>
<td>Fe (+0.5%), Na (0%), V (−0.3%), W (0%)</td>
<td>Al (0%), Cu (−1%), Rh (0%)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>bcc(100)</td>
<td>Fe (+5%), Mo (+9.5%), Ta (−11%), V (−7%), W (−9%)</td>
<td>Al (−8.5%), Ag (−8%), Cu (−8.5%), Ni (−8.5%), Pb (−16%)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>fcc(110)</td>
<td>Be (−17%)</td>
<td>Fe (−15%), W (−12%)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>hcp(10-10)</td>
<td>Re (−17%)</td>
<td>Fe (−15%), W (−12%)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>fcc(311)</td>
<td>Al (−13%), Ni (−16%), Cu (−5%)</td>
<td>Fe (−19%)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>bcc(311)</td>
<td>Al (−12%)</td>
<td>Fe (−19%)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>fcc(210)</td>
<td>Al (−15.5%)</td>
<td>Fe (−17%)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>bcc(310)</td>
<td>Fe (−17%)</td>
<td>Fe (−23%)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Each entry consists of:
Chemical symbol (interlayer spacing change from bulk value).


http://www.tms.org/pubs/journals/JOM/9704/Bulatov/Bulatov-9704.html

Figure 1. The ions in a 552 ion cluster of LaF$_3$ are allowed to move, subject to the forces from all other ions in the nanocluster, until the target temperature of 10 K is reached.

Figure 2. Cross-section view of the ion movement depicted in Figure 1.

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**Relaxation: NaCl(001)**

http://www.molecularuniverse.com/Bound/bound1.htm

A sodium chloride (NaCl) surface. There is a slight rearrangement of the surface: sodium ions move into the surface and chloride ions relax away from the surface.
Surface Reconstruction

- **Si(100)**
- **Si(111)**

Diamond (111), with and without H

- diamond(111)-(1x1)H
- diamond(111)-(2x1)

Bulk termination
Reconstructed
**Surface energy**

- All surfaces are energetically unfavorable because they have a positive free energy of formation with respect to the bulk crystal
  - Bonds must be broken to form the surface
- Surface energy is minimized by:
  - Reducing the amount of exposed surface area
  - Exposing surface planes with low surface tension
  - Altering local atomic geometry (relaxation and reconstruction)
- Low surface energy=high surface stability

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**Rules of thumb for low surface energies (in vacum)**

- High surface atom density
- High coordination number

Arrange these surfaces from lowest to highest stability.
Surface tension

• Total energy: \( U = TS - PV + \mu N + \frac{\partial}{\partial A} \)

• \( \gamma \) = surface tension
  = the reversible work done in forming a unit area of surface
  ≠ surface energy, but lots of people call it that!
  units: energy/area or force/distance (e.g. soap film)

\[ \gamma = \left( \frac{\partial U}{\partial A} \right)_{T,N} \]

We can derive the following relations (Zangwill):

\[ S_s = A \left( \frac{\partial \gamma}{\partial T} \right)_V \]

\( \gamma \) = surface tension
\( T \) = temperature
\( s_{ij} \) = surface stress (force/distance)
\( e_{ij} \) = surface strain

Surface tension is anisotropic in a crystal

• To minimize the excess surface free energy,

\( \int \gamma dA = \text{minimum. But } \int \gamma(hkl) dA(hkl) = \text{minimum.} \)

Wulff construction: easy method for finding the low-temperature equilibrium shape
## Surface tensions of various materials

<table>
<thead>
<tr>
<th>Material</th>
<th>Surface energy (mJ/m²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>W</td>
<td>4400</td>
</tr>
<tr>
<td>Cu</td>
<td>2000</td>
</tr>
<tr>
<td>Ag</td>
<td>1500</td>
</tr>
<tr>
<td>Al</td>
<td>1100</td>
</tr>
<tr>
<td>Water</td>
<td>73</td>
</tr>
<tr>
<td>Ethanol</td>
<td>22.8</td>
</tr>
<tr>
<td>Teflon</td>
<td>18.3</td>
</tr>
</tbody>
</table>

from Israelachvili, “Intermolecular and Surface Forces”

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## Summary