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Thin Coating Contact Mechanics with Adhesion

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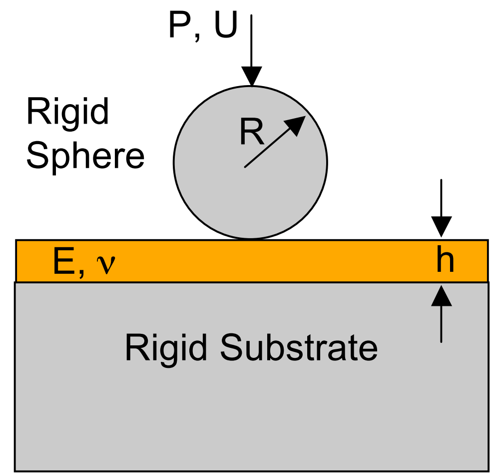
Thin Coating Contact Mechanics Theory

<u>Model definition:</u>

- Rigid spherical indenter with radius *R*.
- Thin coating with thickness *h* is fully bonded to a flat, rigid substrate ($h/R << 1$).
- Coating is linear elastic and the material is compressible (i.e., $\nu \le 0.45$).
- a/R << 1 and $a/h >> 1$, where *a* is contact radius.
- Small strains and frictionless contact.
- Assume deformation through the coating is homogeneous; normal compressive stress σ_z, radial stress σ_r and and hoop stress σ_θ are all uniform through the thickness.
- The contact radius and the compressive strain ε_z are determined by the geometry of the indenter. For indenter approach *U*,

$$\varepsilon_z(r) = \frac{a^2}{2Rh}\left(1 - \left(\frac{r}{a}\right)^2\right)$$

where $a^2 = 2RU$.



- Compressive stress $\sigma_z = E_u\,\varepsilon_z$ where E_u is the uniaxial strain modulus ($\varepsilon_r = \varepsilon_\theta = 0$).

$$E_u = \frac{(1-\nu)E}{(1+\nu)(1-2\nu)}$$

- The applied compressive load *P* is determined by integrating the compressive stress over the contact area.

$$P = \frac{\pi E_u a^4}{4Rh} = \frac{E_u A^2}{4\pi Rh} = \frac{\pi E_u R U^2}{h}$$

where *A* is the contact area.

Thin Coating Contact Mechanics Theory

- Thin coating contact theory results can be expressed in nondimensional form

$$\overline{A} = 2\sqrt{\pi}\,\overline{P}^{1/2}$$

where

$$\overline{A} = \frac{A}{Rh} \text{ and } \overline{P} = \left(\frac{P}{RhE_u}\right)$$

- The thin coating contact theory can be formally extended to cases where h/R and a/R are not vanishing small (but still relatively small) by assuming that

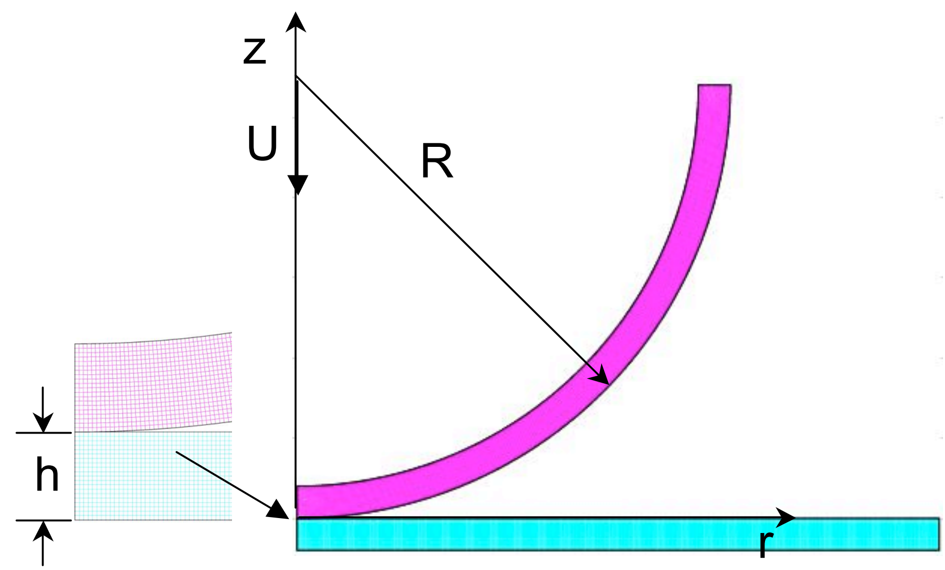
$$\overline{A} = 2\sqrt{\pi}\,c\,\overline{P}^{\,d}$$

where in the thin coating limit $c=1$ and $d = 1/2$.

- Based on dimensional considerations, one anticipates that the parameters c and d are functions of ν and h/R.

Finite Element Contact Simulations for a Thin Coating

- Used SNL's Tahoe finite element code.
- Quasistatic, small strain, axisymmetric, linear elastic analysis.
- Frictionless contact of spherical shell of radius *R* on a thin coating of thickness *h*.
- Modulus of spherical shell is 10^6 times that of the elastic coating => shell is essentially rigid.
- Bottom edge of elastic layer fixed to model bond to a rigid substrate.
- Analysis for *U/h*<0.2; small strain, linear elastic analysis is problematic when *U/h gets large.*



elastic coating fixed on bottom edge.

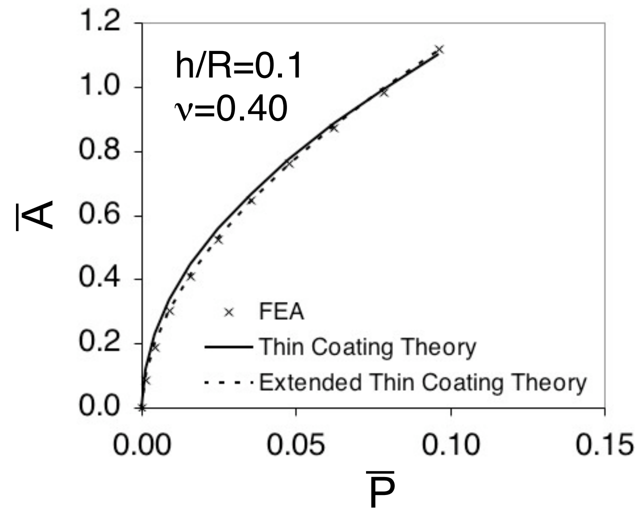
•Elements are 0.1 nm squares.

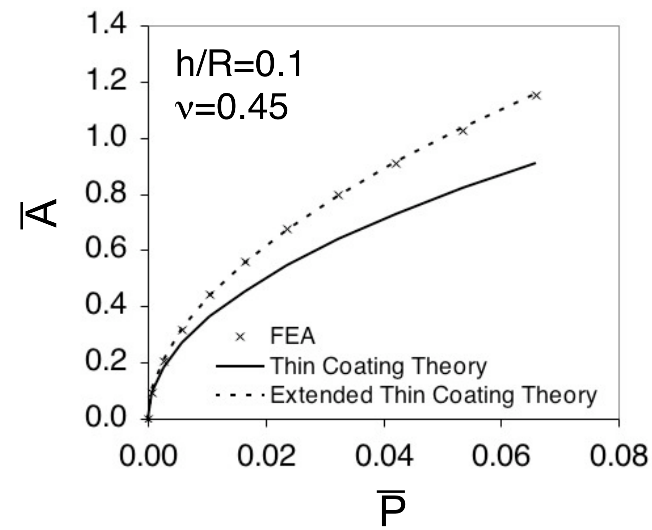
•Spherical shell displacement U is downward.

Finite Element Contact Simulations for a Thin Coating

ν	parameters	h/R =0.010	h/R =0.038	h/R =0.074	h/R =0.100
0.00	c=	1.01	0.97	0.93	0.93
	d=	0.53	0.54	0.55	0.56
0.10	c=	1.00	0.97	0.94	0.94
	d=	0.52	0.54	0.55	0.57
0.20	c=	1.02	0.99	0.93	0.94
	d=	0.53	0.54	0.54	0.56
0.30	c=	1.02	1.01	0.99	0.97
	d=	0.52	0.54	0.55	0.55
0.40	c=	1.05	1.10	1.11	1.13
	d=	0.50	0.52	0.53	0.55
0.45	c=	1.17	1.27	1.33	1.38
	d=	0.49	0.50	0.52	0.53

Fits for a/h>1 and U/h<0.2

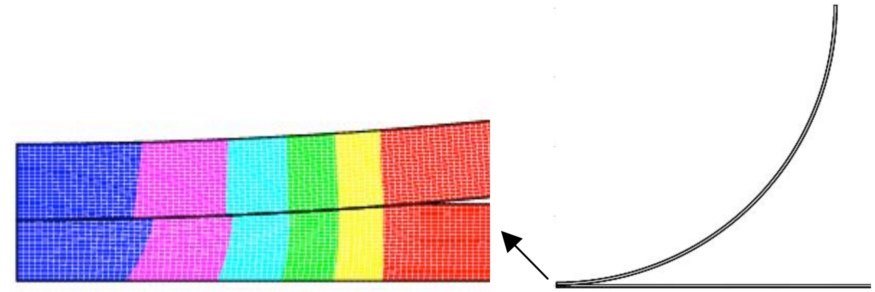




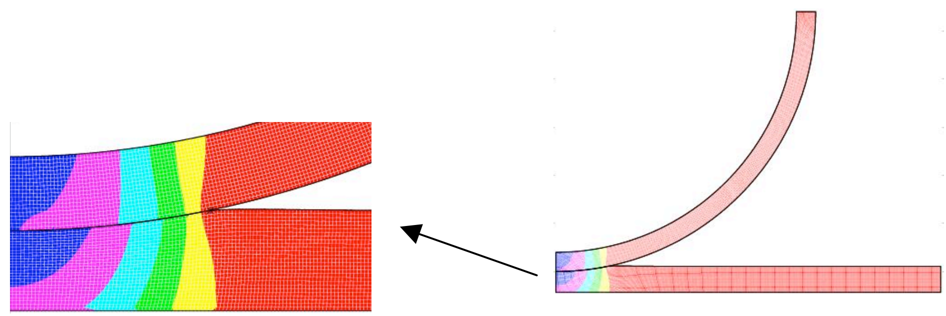
- Performed a suite of finite element analyses with
  - determined power law fit parameters *c, d* in $\bar{A} = 2\sqrt{\pi c}\bar{P}^{d}$
- Thin coating contact theory is a reasonable approximation to the FEA for most parameter combinations (e.g. *h/R*=0.1, ν=0.4).
- The greatest deviation from thin coating contact theory occurs as h/R increases and for ν>0.4 (e.g., *h/R*=0.1, ν=0.45).
- The extended thin coating theory provides a good fit to the FEA for the full range of *h/R* and ν considered.

Finite Element Contact Simulations for a Thin Coating

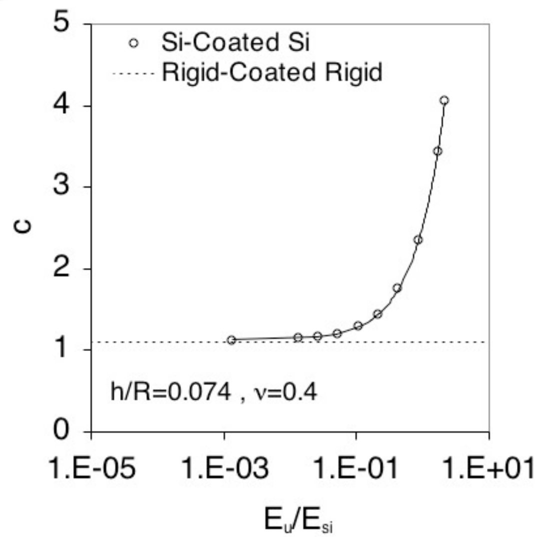
- Expect thin coating theory assumptions apply when $h/R=0.01$ and $\nu=0.4$.
- FEA contour plot of normal stress for $U/h=0.2$ shows that the normal stress is nearly uniform through the coating thickness.
- In this case fit parameters $c=1.05$ and $d=0.50$.

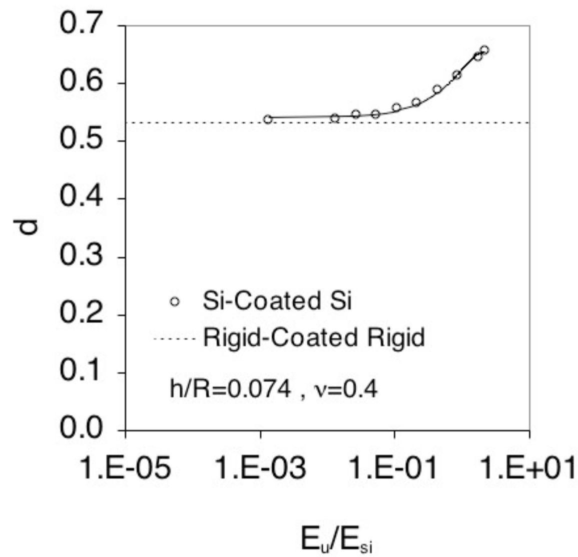


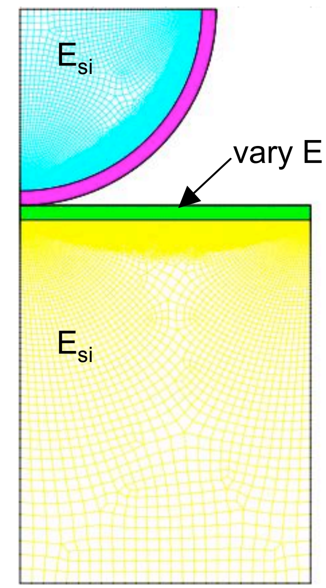
- Expect some deviation form thin coating theory assumptions when $h/R=0.1$ and $\nu=0.45$.
- FEA contour plot of normal stress for $U/h=0.2$ shows that the normal stress exhibits some variation through the coating thickness.
- In this case fit parameters $c=1.38$ and $d=0.53$.



Finite Element Contact Simulations for a Thin Coating







- Performed a suite of axisymmetric finite element calculations to examine when the rigid indenter/substrate idealization is applicable.
- Indenter and substrate have elastic properties similar to silicon (E_{si}=161 GPa, ν_{si}= 0.23).
- Elastic modulus of the elastic layer is varied from E=0.1 GPa to 161 GPa (v=0.4).
- Performed calculations for h/R = 0.074.
- Simulations suggest that the rigid indentor/substrate idealization is reasonable when E_u/E_{si} < 0.05.

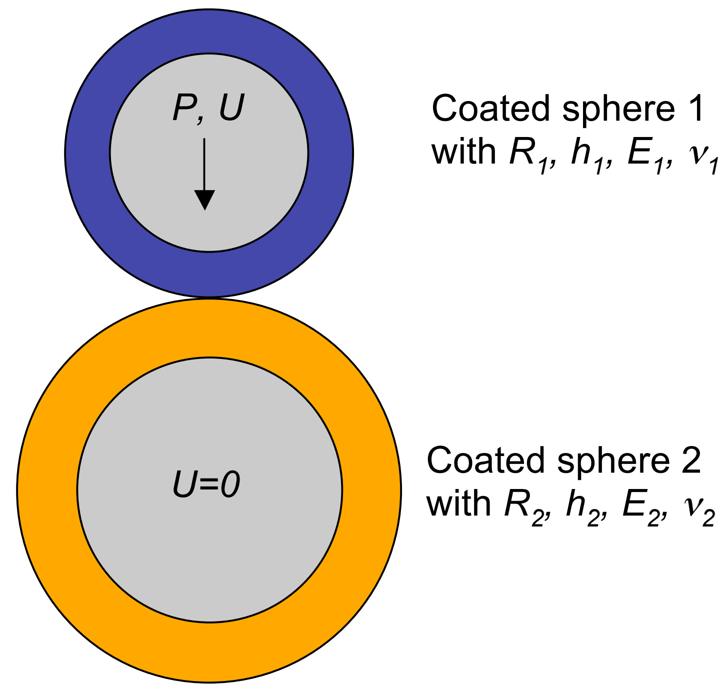
Thin Coating Contact Mechanics Theory

- Can readily extend to two contacting spheres, where each sphere is rigid and coated with a thin compliant elastic material by using an effective R and E_u.
- Based upon the assumed kinematics of the deformation (i.e., the sum of the imposed normal coating deformation is equal to the approach minus the initial gap) the effective radius is

$$R = \left(1/R_1 + 1/R_2\right)^{-1}$$

- Based upon the assumptions of uniaxial strain and uniform, through the thickness normal stress σ_z, a two material stack can be replace by a single material with effective modulus of

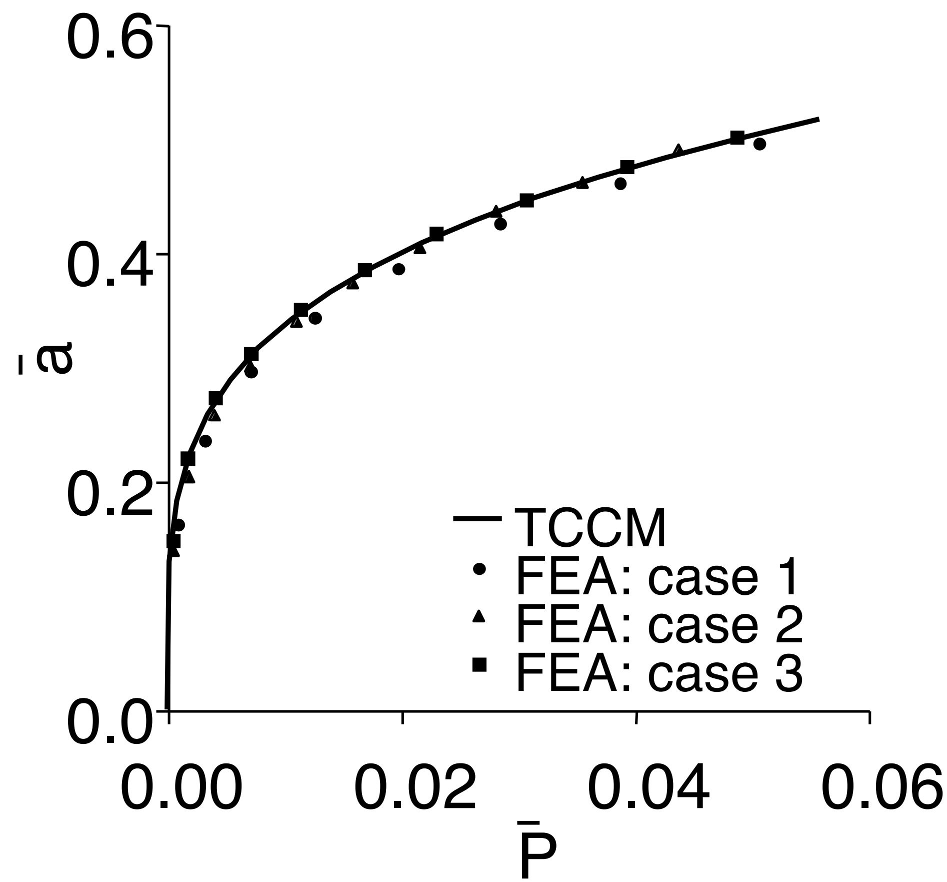
$$E_u = h\left(h_1/E_{u1} + h_2/E_{u2}\right)^{-1} \text{where} \quad h = h_1 + h_2$$



R_i = coating radius
h_i = coating thickness
E_i = coating Young's modulus
ν_i = coating Poisson's ratio

Thin Coating Contact Mechanics: Illustrative Results

	Case 1	Case 2	Case 3
R_1 (nm)	52	52	200
h_1 (nm)	2	2	2
E_1 (MPa)	∞	2000	4000
ν_1	na	0.3	0.4
R_2 (nm)	∞	∞	1000
h_2 (nm)	4	4	2
E_2 (MPa)	1000	4000	4000
ν_2	0.4	0.4	0.4



- Results from all three cases collapse to the universal TCCM relationship for Hertz-like response.

DMT-like Thin Coating Contact Mechanics Theory

- DMT-like theory
  - -Hertz-like contact with adhesion forces acting outside of the contact radius.
  - -Adhesion does not deform the contacting materials outside of the contact zone.
  - -Most appropriate when range of adhesion forces long compared with elastic deformations (W/E_u relatively small).
- The total load equals the sum of the applied compressive load P and the load induced by adhesion $P_{a\,(DMT)}$.
- $P_{a\,(DMT)} = 2\pi RW$ where W is the work of adhesion (the force between a rigid sphere and a rigid half-plane).
- Consequently, using the thin coating contact mechanics theory results,

$$P + 2\pi RW = \frac{\pi E_u a^4}{4Rh} = \frac{E_u A^2}{4\pi Rh} = \frac{\pi E_u RU^2}{h}$$

- Can nondimensionalize equations using:

$$\bar{P} = \frac{P}{E_u Rh} \quad \bar{U} = \frac{U}{\sqrt{Rh}} \quad \bar{a} = \frac{a}{\sqrt{Rh}}$$

$$\bar{W} = \frac{W}{E_u h} \quad \bar{h} = \frac{h}{\sqrt{Rh}}$$

- So $$\bar{P} + 2\pi\bar{W} = \frac{\pi\bar{a}^4}{4}$$

and $$\bar{a} = \left(\frac{2\bar{U}}{\bar{h}}\right)^{1/2}$$

and $$\bar{P} + 2\pi\bar{W} = \pi\left(\frac{\bar{U}}{\bar{h}}\right)^2$$

- When $\bar{U} = 0$

$$\bar{a} = 0 \qquad \bar{P} = -2\pi\bar{W}$$

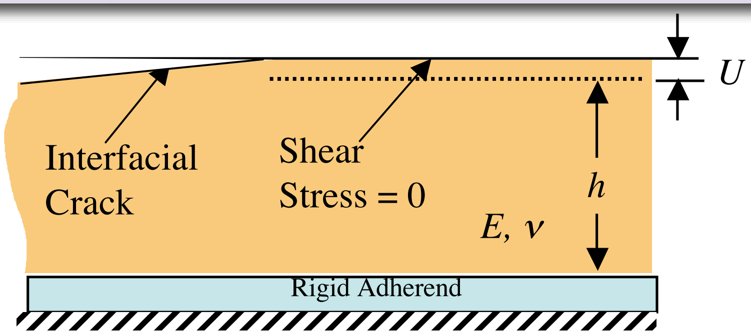
which is the tensile pull-off load.

- When $\bar{P} = 0$

$$\bar{a} = \left(8\bar{W}\right)^{1/4} \qquad \bar{U} = \bar{h}\left(2\bar{W}\right)^{1/2}$$

JKR-like Thin Coating Contact Mechanics Theory

- JKR-like theory
  - -Adhesion induced elastic deformations included.
  - -Adhesion forces act only within contact area.
  - -Most appropriate when range of adhesion forces short compared with elastic deformations (W/E_u relatively large).
- The applied contact load is the sum of compressive load corresponding to a contact radius a minus the load P_a induced by adhesion.
- For a thin compliant coating on a flat rigid substrate indented by a rigid sphere with $R/h>>1$, $R/a>>1$, and $a/h>>1$, the adhesion problem can be idealized as an edge-clamped thin strip.



- Note that a plane-strain-like condition applies since the bottom edge is fixed with $u_r = \varepsilon_\theta = 0$, so a J-integral evaluation yields

$$J = \frac{hE_u}{2}\left(\frac{U}{h}\right)^2 = \frac{\sigma_o{}^2 h}{2E_u}$$

where σ_o is the nominal normal stress in the uncracked portion of the strip

- Since $J = W$ when the materials are linear elastic,

$$\sigma_o = \left(\frac{2WE_u}{h}\right)^{1/2}$$

- Since most of the strip is subjected to σ_o when $a/h>>1$, will assume that

$$P_{a\,(JKR)} = \pi a^2\left(\frac{2E_u W}{h}\right)^{1/2}$$

and consequently the net contact force is

$$P = \frac{\pi a^4 E_u}{4Rh} - \pi a^2\left(\frac{2E_u W}{h}\right)^{1/2}$$

JKR-like Thin Coating Contact Mechanics Theory

- The applied displacement is the sum of of the displacement corresponding to a contact radius *a* minus the displacement $U_{a\,(JKR)}$ induced by adhesion.

- Since

$$J = W = \frac{hE_u}{2}\left(\frac{U_{a\,(JKR)}}{h}\right)^2$$

then the net displacement is

$$U = \frac{a^2}{2R} - \left(\frac{2Wh}{E_u}\right)^{1/2}$$

- The nondimensionalized JKR-like thin coating are

$$\overline{P} = \frac{\pi}{4}\overline{a}^4 - \pi\overline{a}^2\left(2\overline{W}\right)^{1/2}$$

$$\overline{a} = \left(\frac{2\overline{U}}{\overline{h}} + \left(8\overline{W}\right)^{1/2}\right)^{1/2}$$

- These equations can be solved to yield

$$\overline{P} + 2\pi\overline{W} = \pi\left(\frac{\overline{U}}{\overline{h}}\right)^2$$

Which is identical to the DMT result, but here $\overline{U}$ can be negative as long as $\overline{a} \geq 0$.

- When $\overline{U} = 0$

$$\overline{P} = -2\pi\overline{W}$$

$$\overline{a} = \left(8\overline{W}\right)^{1/4}$$

The maximum tensile load occurs when *U=0*, thus defining the value of the pull-off force for a tensile loading.

- When $\overline{P} = 0$

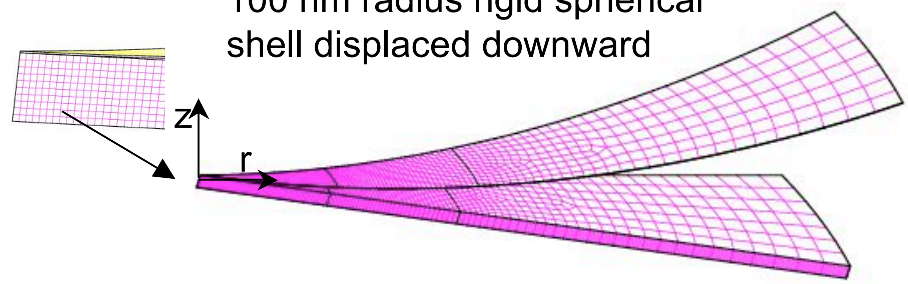
$$\overline{U} = \overline{h}\left(2\overline{W}\right)^{1/2}$$

$$\overline{a} = \left(32\overline{W}\right)^{1/4}$$

Finite Element Simulations that Include Adhesion

- Used SNL's PRESTO 3-D, explicit dynamics finite element code.
- Adhesion model combines frictionless contact with an adhesion traction that scales with normal distance between opposing surfaces (implemented via the contact algorithm).
- Large strain and displacement analysis --- if no material rotation at a point logarithmic strain.
- Begin analysis with rigid sphere just in contact with top of elastic coating (*U=0*).
- Adhesion rapidly pulls coating into contact --- hold sphere fixed until contact radius has reached its equilibrium position (analysis includes viscous damping).
- Next slowly displace rigid sphere (push or pull) to determine relationship between contact radius and applied load (1nm/ns).

100 nm radius rigid spherical shell displaced downward

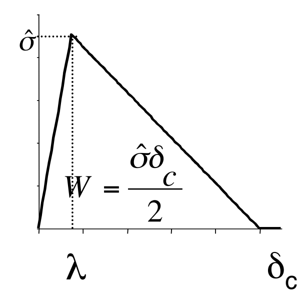


1 nm thick elastic coating fixed on bottom edge

•Smallest element is a 0.1 nm cube.

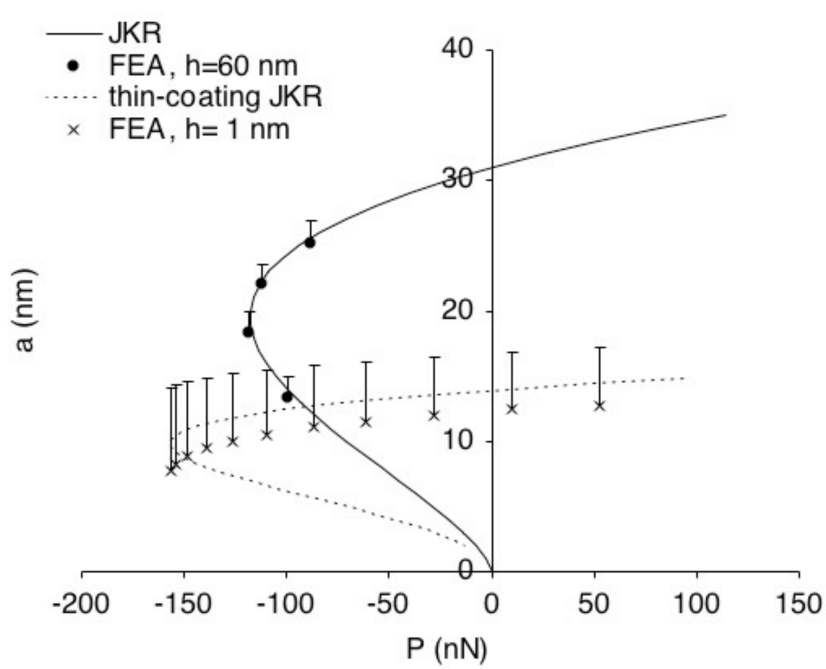
- Results of test calculations with a refined mesh (0.05 nm cube) were essentially the same.
- If mesh is too coarse or when $\hat{\sigma}$ is comparable to E, can have element stability issues.

Adhesion traction-separation relationship



Note: $\lambda \leq 0.001$ in finite element calculations (consistent with the cracked strip problem used in the JKR-like analysis).

Thin Coating Contact Mechanics: Illustrative Results

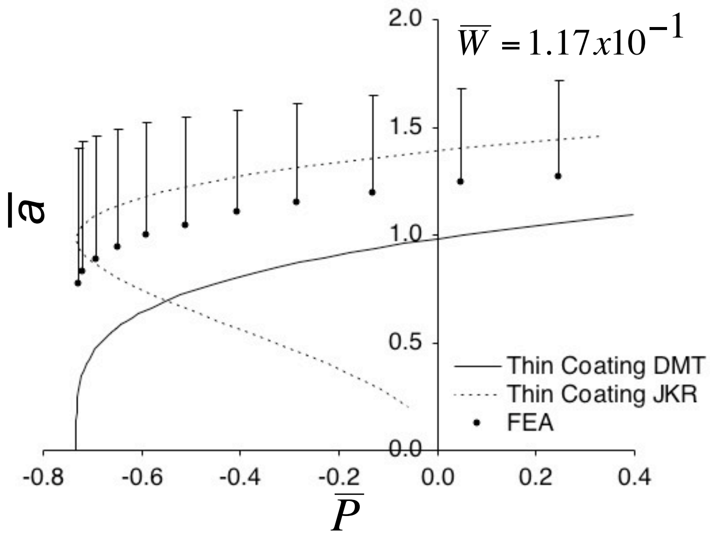


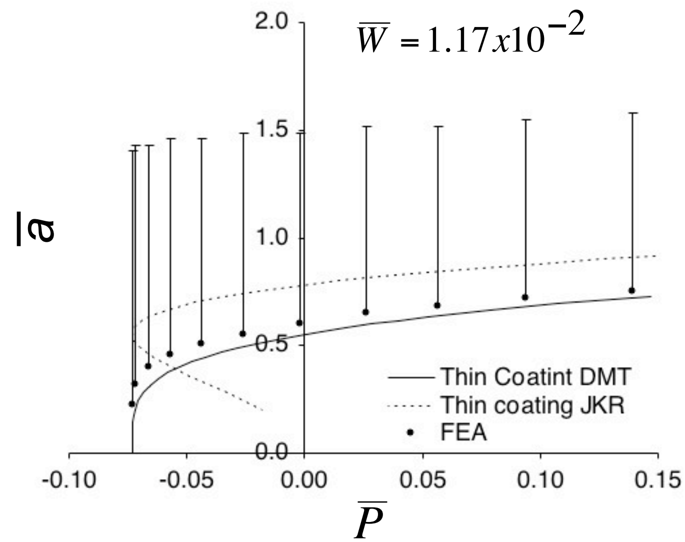
Note: symbol denotes contact radius, bar indicates length of zone where adhesion forces act across an open gap

- Illustrative calculations with:
  - *R* =100 nm, *E* =1 GPa, ν = 0.4, ρ = 1 g/cm^3
  - *W* = 0.25 J/m^2, $\hat{\sigma}$ = 500 MPa, δ_c=1 nm
  - Either a thin coating with *h=1 nm* or a thick substrate with h= 60 nm (should be JKR-like).

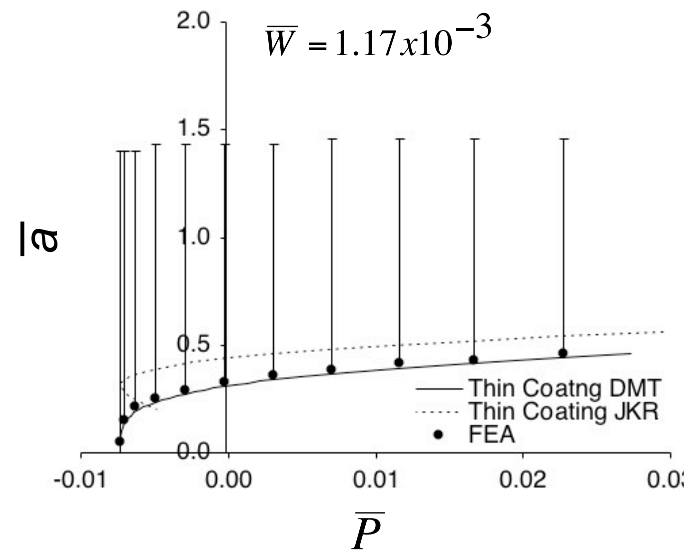
- Contact radius is defined as the radius where the stress equals $\hat{\sigma}$.
- When there is a thick substrate:
  - Finite element analysis (FEA) is in good agreement with JKR theory.
  - Calculated zone where adhesion forces act across an open gap is relatively short compared with the contact radius.
  - Note that the FEA uses a simple adhesion model and does not assume JKR behavior.
- In comparison with a thick substrate, a thin coating has:
  - a much smaller contact radius for a given contact force.
  - a much larger tensile pull-off force.
  - a relatively large adhesive zone.
- FEA results for a thin film
  - predict pull off at *U=0* with $P=-2\pi RW$ and $a/h \sim 10$ (consistent with JKR-like theory).
  - predicted adhesive zone length bounds the TCCM JKR theory prediction for *a*.

Thin Coating Contact Mechanics: Illustrative Results





- Illustrative calculations
  - *R =100 nm, h=1 nm*
  - ***E =1, 10, or 100 GPa****, ν = 0.4, ρ = 1 g/cm³*
  - *W = 0.25 J/m², $\hat{\sigma}$ = 500 MPa, δ_c=1 nm*
- Approaches the thin coating DMT limit as $\overline{W} = W/(E_u h)$ decreases.
- Adhesive zone length can be quite large compared to the contact radius in the thin coating DMT limit.
- Tensile pull-off load is within 1% of *-2πRW* for all three cases.



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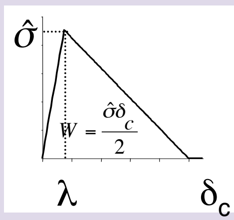
TCCM: transition between DMT-like and JKR-like limits

- Within the context of TCCM, the coating strain is assumed to be uniaxial and uniform through the coating thickness while the Adhesion-Separation relationship defines the peak adhesive stress $\hat{\sigma}$.



- Consequently the adhesion induced coating displacement U_a is simply

$$U_a = \hat{\sigma}h / E_u = 2\bar{W}h^2 / \delta_c$$

  - used W=$\hat{\sigma}\delta_c$/2 above
  - U_a is the maximum gap that adhesion can close-up.
  - note that in the JKR-like limit, $U_a = \delta_c$ (no adhesion outside of the contact zone).

- Can define a thin-coating transition parameter ζ.

$$\zeta = \frac{U_a}{\delta_c} = \frac{2Wh}{E_u \delta_c^2} = 2\bar{W}\left(\frac{\bar{h}}{\delta_c}\right)^2$$

  - when $\zeta = 0$, DMT-like, when $\zeta = 1$ JKR-like.
  - when $\zeta < 1$, adhesion force acts across an open gap.

- Recall results for the DMT-like and JKR-like limits

$$\frac{\bar{a}^2}{2} = \frac{\bar{U}}{\bar{h}} \quad \text{DMT-like}$$

$$\frac{\bar{a}^2}{2} = \frac{\bar{U}}{\bar{h}} + \left(2\bar{W}\right)^{1/2} \quad \text{JKR-like}$$

- These equations differ only by a load and contact radius independent quantity that depends on adhesion, $\left(2\bar{W}\right)^{1/2}$.
- This suggests that a function that depends only on ζ, $f(\zeta)$, can be defined to span the DMT-like to JKR-like limits

$$\frac{\bar{a}^2}{2} = \frac{\bar{U}}{\bar{h}} + f(\zeta)\left(2\bar{W}\right)^{1/2}$$

where $f(\zeta) = 0$ when $\zeta = 0$ (DMT-like)

and $f(\zeta) = 1$ when $\zeta = 1$ (JKR-like).

- Now since $\left(2\bar{W}\right)^{1/2} = \zeta^{1/2}\delta_c / h$ (using W=$\hat{\sigma}\delta_c$/2)

$$\frac{\bar{a}^2}{2} = \frac{\bar{U}}{\bar{h}} + f(\zeta)\zeta^{1/2}\frac{\bar{\delta}_c}{\bar{h}}$$

TCCM: transition between DMT-like and JKR-like limits

- When $\overline{U} = 0$

$$\frac{\overline{a}_o^2}{2} = f(\zeta)\zeta^{1/2}\frac{\overline{\delta}_c}{\overline{h}}$$

where a_0 is the contact radius when $U = 0$ and $\overline{\delta}_c = \delta_c / \sqrt{R/h}$.

- Next note that when $U=0$, the displacement associated with Hertz-like contact equals that induced by adhesion so that

$$\frac{\overline{a}_o{}^2}{2} = \frac{\overline{U}_a}{\overline{h}} = \frac{\overline{U}_a}{\overline{\delta}_c}\frac{\overline{\delta}_c}{\overline{h}} = \zeta\frac{\overline{\delta}_c}{\overline{h}}$$

- Comparison of the two equations suggest that

$$f(\zeta) = \zeta^{1/2}$$

- Using this result along with the TCCM relationship (same for DMT-like and JRK-like limits)

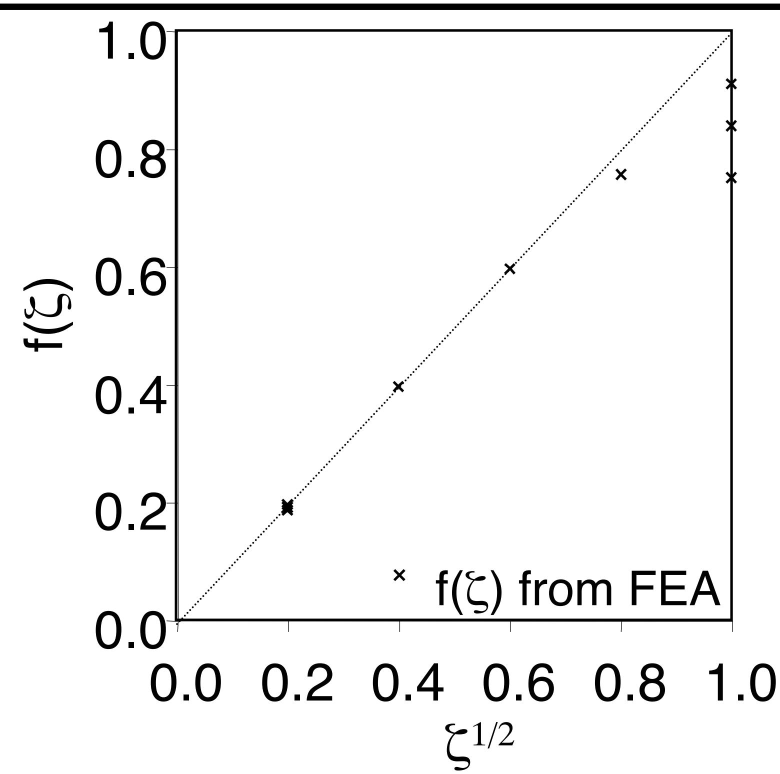
$$\overline{P} + 2\pi\overline{W} = \pi\left(\frac{\overline{U}}{\overline{h}}\right)^2$$

gives

$$\overline{P} = \frac{\pi}{4}\overline{a}^4 - \zeta^{1/2}\pi\overline{a}^2(2\overline{W})^{1/2} - 2\pi\overline{W}(1-\zeta)$$

Finite element calculations verify $f(\zeta) = \zeta^{1/2}$

R (nm)	h (nm)	W (J/m²)	$\hat{\sigma}/E_u$	a_o/h	$\zeta^{1/2}$	f(ζ)
100	1	0.050	0.04	2.8	0.2	0.191
200	1	0.050	0.04	4.0	0.2	0.196
200	2	0.025	0.02	1.9	0.2	0.186
200	2	0.100	0.08	4.0	0.4	0.395
200	3	0.150	0.12	4.0	0.6	0.595
200	4	0.200	0.16	3.9	0.8	0.755
400	10	0.125	0.10	2.5	1.0	0.749
1250	10	0.125	0.10	4.6	1.0	0.838
5000	10	0.125	0.10	9.5	1.0	0.909

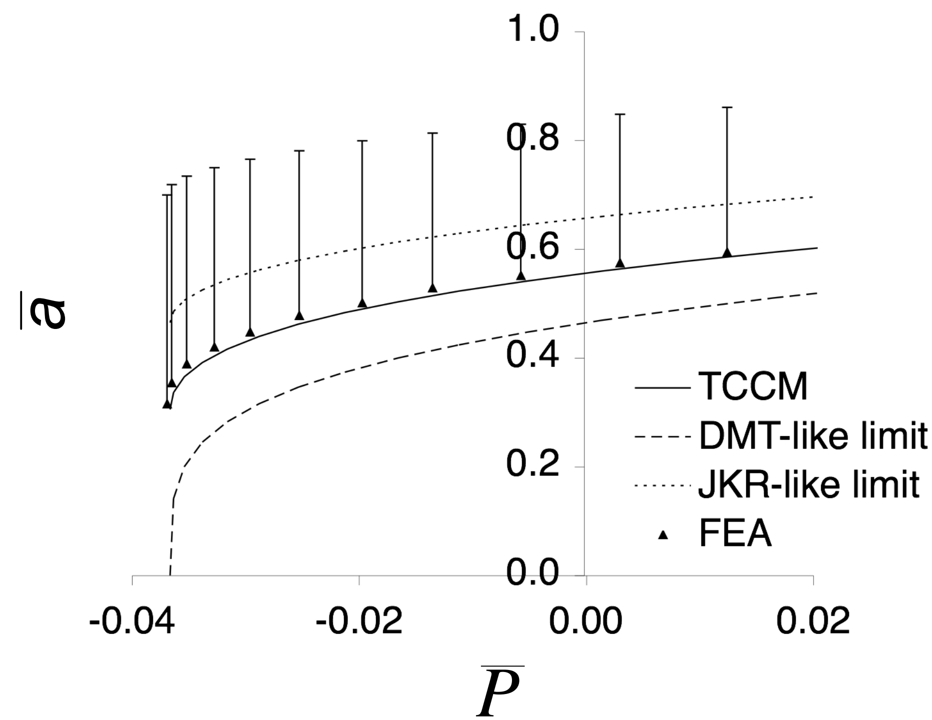


- Calculations for a rigid sphere of radius *R* contacting a coating of thickness *h*. Used calculated a_o to determine $f(\zeta)$
- E_u = 2490 MPa, δ_c = 1 nm
- $h/R < 0.025$, $a_o/R < 0.08$,

- $\hat{\sigma}/E_u < 0.16$($\hat{\sigma}/E_u$ is a measure of the maximum, nominal tensile coating strain ---TCCM assumes small strain, linear elasticity)
- When ζ=1, need $a_o/h \geq 10$ to approach $f(\zeta) = \zeta^{1/2}$ (TCCM assumes *a/h>>1*). It appears that a_o/h can be much less than10 for smaller values of ζ (when "displacement discontinuity" at contact radius is less severe).

Thin Coating Contact Mechanics: Example Problem

- Example problem: two coated spheres with adhesion
  - Sphere 1: R_1 = 200 nm
  - Sphere 2: R_2 = 1000 nm
  - W = 0.2 J/m^2 (δ_c = 1 nm)
  - Both spheres have a 2-nm thick coating with E = 4 GPa and ν = 0.4
  - ζ = 0.19
  - $\hat{\sigma} / E_u = 0.047$
  - a/h =2.0 when U = 0.
  - Symbols denote the contact radius while the bars indicate the length of the region where adhesion forces act across an open gap.



Summary

- Developed an elementary thin coating contact mechanics theory for two contacting spheres, where each sphere is rigid and coated with a thin compliant elastic material (use an effective R and E_u).
- Performed axisymmetric finite element simulations to assess the range of validity of the thin coating contact mechanics theory and defined an extension based on the FEA results.
- Derived DMT-like and JKR-like thin coating contact mechanics limits and also provide analytical results that span the transition between the DMT-like and JKR-like limits.
- Developed a 3-D finite element simulation capability that includes adhesion and verified that this FEA can reproduce JKR-like response when there is a thick, compliant substrate.
- Performed illustrative FEA for a thin compliant coating with adhesion (rigid indenter/substrate) and compared results with the thin coating contact theory.

Summary of TCCM governing equations

TCCM governing equations

$$\bar{P} = \frac{\pi}{4}\bar{a}^4 - \zeta^{1/2}\pi\bar{a}^2(2\bar{W})^{1/2} - 2\pi\bar{W}(1-\zeta)$$

$$\frac{\bar{a}^2}{2} = \frac{\bar{U}}{\bar{h}} + \left(2\zeta\bar{W}\right)^{1/2}$$

$$\bar{P} + 2\pi\bar{W} = \pi\left(\frac{\bar{U}}{\bar{h}}\right)^2$$

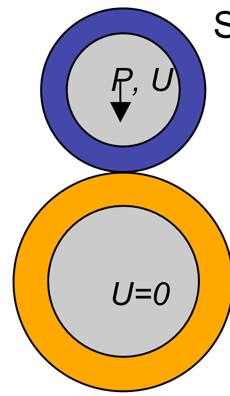
$$\zeta = 2\bar{W}\left(\frac{\bar{h}}{\bar{\delta}_c}\right)^2$$ Transition parameter

NOTE: $\bar{P} = \frac{P}{E_u R h}$ $\quad \bar{U} = \frac{U}{\sqrt{Rh}}$ $\quad \bar{a} = \frac{a}{\sqrt{Rh}}$

$\bar{W} = \frac{W}{E_u h}$ $\quad \bar{h} = \frac{h}{\sqrt{Rh}}$ $\quad \bar{\delta}_c = \frac{\delta_c}{\sqrt{Rh}}$

where $E_u = \frac{(1-\nu)E}{(1+\nu)(1-2\nu)}$

Sphere 1 with R_1, h_1, E_1, ν_1



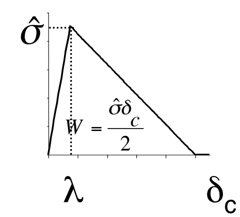
Sphere 2 with R_2, h_2, E_2, ν_2

$$R = \left(1/R_1 + 1/R_2\right)^{-1}$$

$$E_u = h\left(h_1/E_{u1} + h_2/E_{u2}\right)^{-1}$$

where $h = h_1 + h_2$

Adhesion traction-separation relationship



- Thin coating is fully bonded to a rigid sphere (*h/R << 1)*.
- Coating is linear elastic and the material is compressible (i.e., $\nu \leq 0.45$).
- a/R << 1 and *a/h >> 1*, where *a* is contact radius.
- Small strains and frictionless contact.