A Model for Undercut Etching

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Introduction

- Undercutting causes particle removal by isotropic etching of the substrate on which the particle adheres
- Adhesion force can be approximated as the sum of the van der Waals force and the electrostatic double layer force
- Particle is removed when the net adhesion force is repulsive

$$F_A = F_{vdW} + F_E$$

Total Adhesion Force

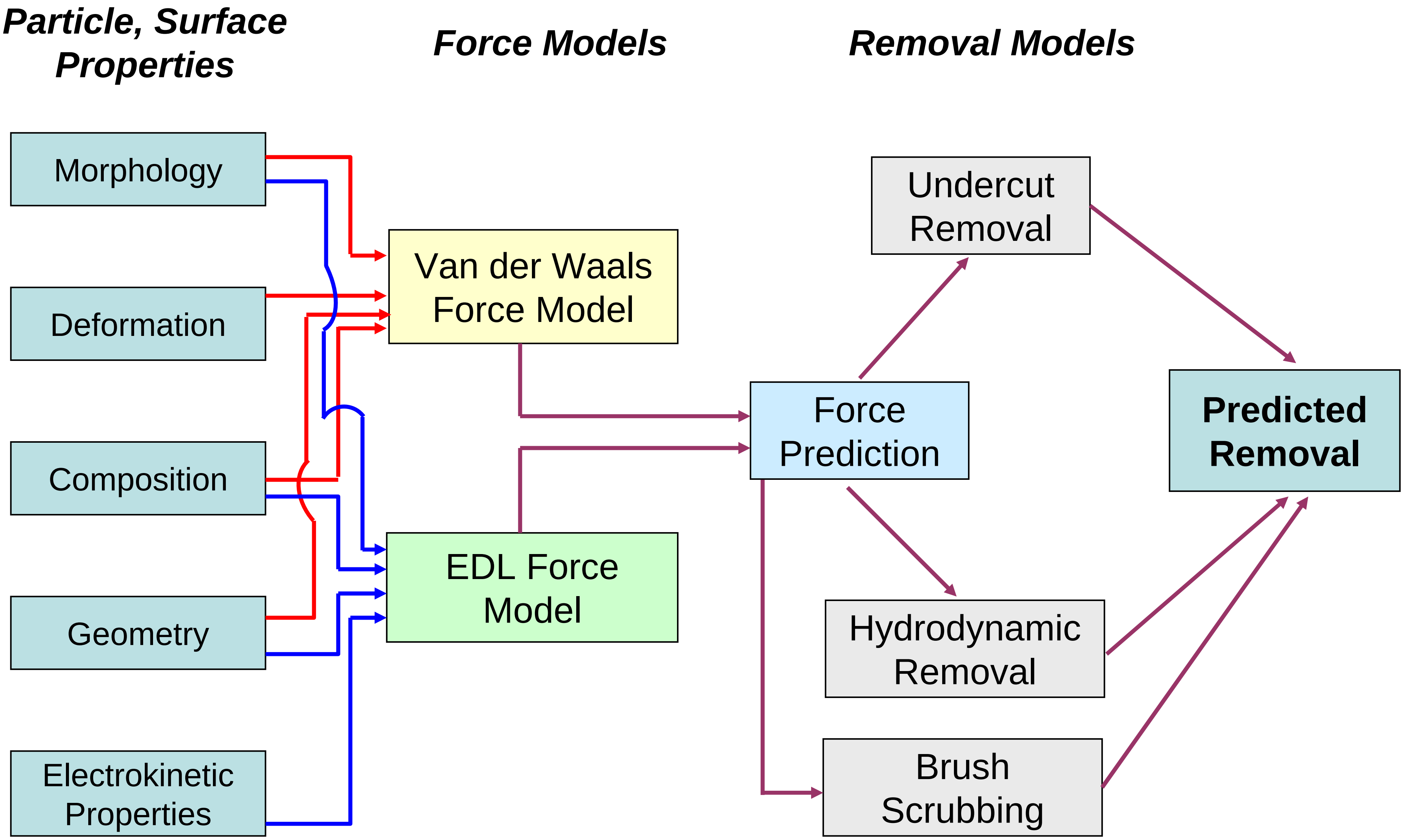
van der Waals Force

Electrostatic Double Layer Force

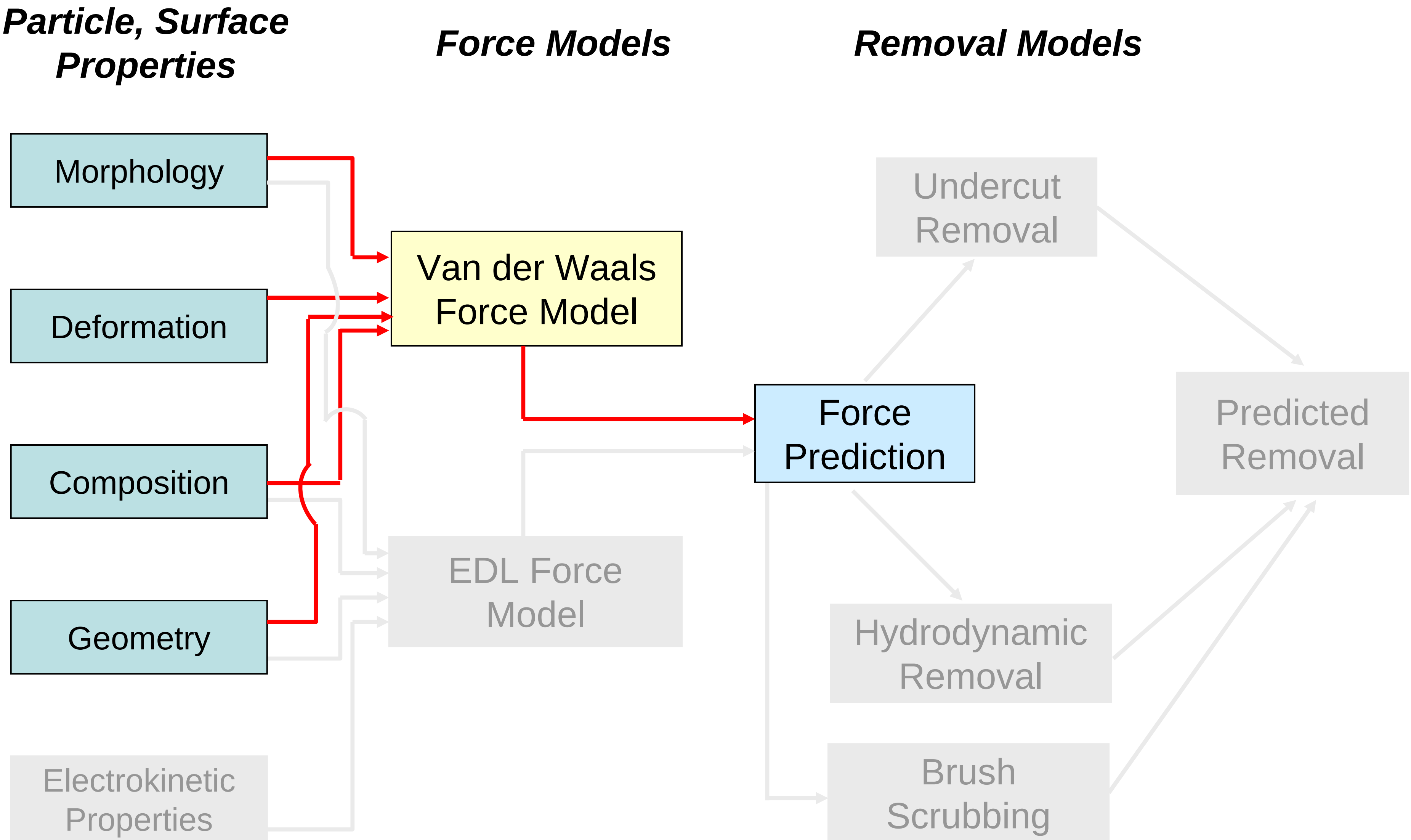
Goal

- Provide a scientific basis for undercut cleaning
  - Interpret cleaning rates in terms of measurable systems parameters
  - Develop general approach such that extension to include hydrodynamics, megasonics possible
  - To facilitate interpretation, focus on model system
    - Micron-scale polystyrene latex adhering to SiO_2

Overall Approach



The van der Waals Force Model



Theory – van der Waals Force

$$F_{vdW} = \frac{A_{132}d}{12h^2}\left(1+\frac{2a^2}{hd}\right)$$

A = System Hamaker constant

d = Particle diameter

a = Contact radius

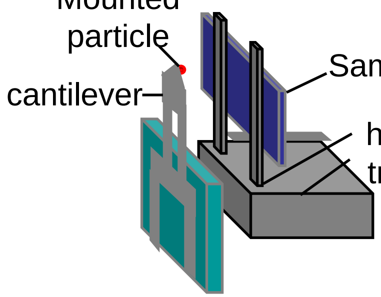
h = Particle-surface separation distance

Validation

Observation
Measure particle/wafer interactions in relevant solutions

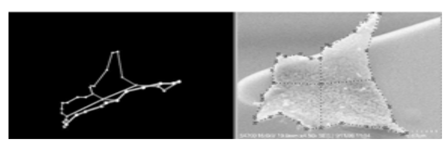
Model Inputs
Identify key properties that control van der Waals force and quantify their effects

Model Prediction
Distribution of forces

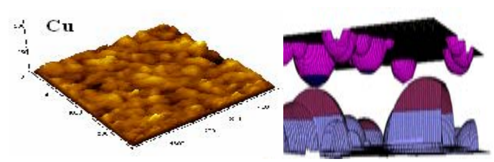


AFM Force Measurements

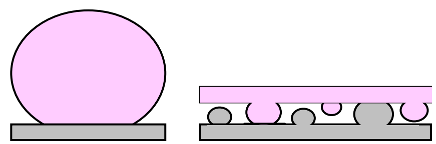
Composition



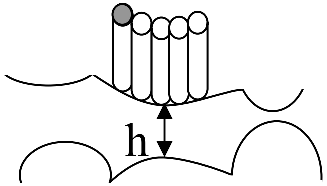
Geometry



Morphology

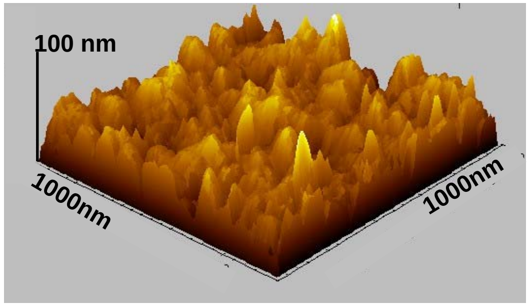


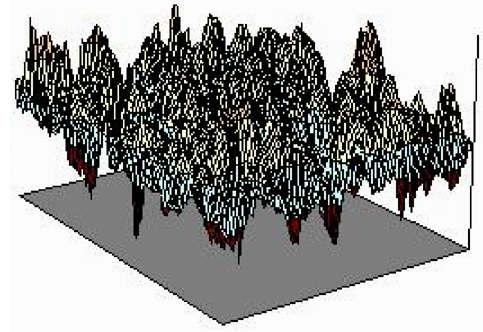
Deformation



van der Waals Model (Integrate vdW force over volume elements)

FFT Model for surfaces





Fourier transform equation:

$$f(k) = \int_{-\infty}^{\infty} f(x) e^{-i2\pi fx} dx$$

Fourier transform of surface profile

$$f(x) = \sum_{k=-\infty}^{\infty} \hat{f}_k e^{ikx}$$

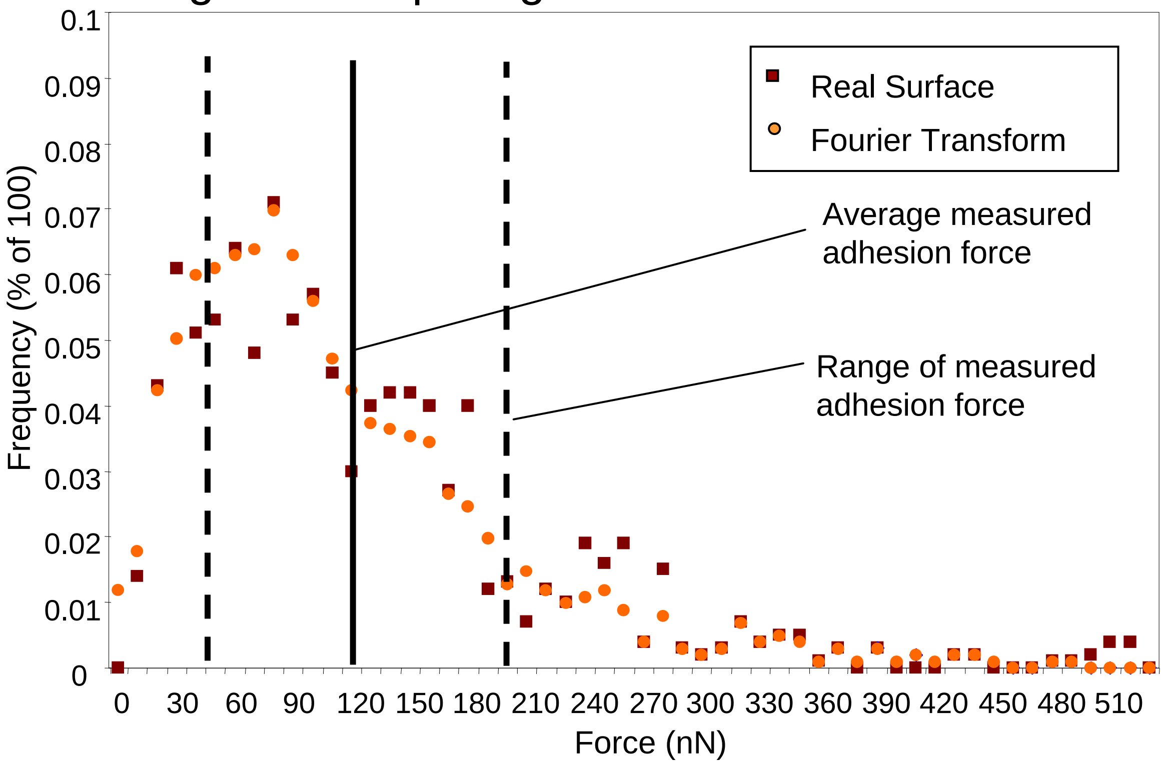
$$\hat{f}_k = \frac{1}{2N} \sum_{j=0}^{2N-1} f(x_j) e^{ikx_j}$$

Addition of random phase angle

$$f(x) = \sum_{k=0}^{n-1} F_k e^{i2\pi\left[\phi_k + \frac{kx}{n}\right]}$$

$$f(x,y) = \sum_{k=0}^{n-1} \sum_{l=0}^{m-1} F_{k,l} e^{i2\pi\left[\phi_{k,l} + \frac{kx}{m} + \frac{ly}{n}\right]}$$

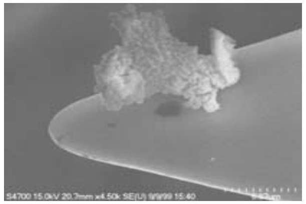
Histogram Comparing Predicted Adhesion Forces



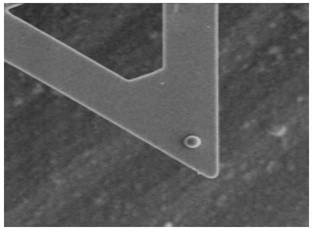
Measurement of van der Waals Force

Particles Mounted on AFM Cantilevers

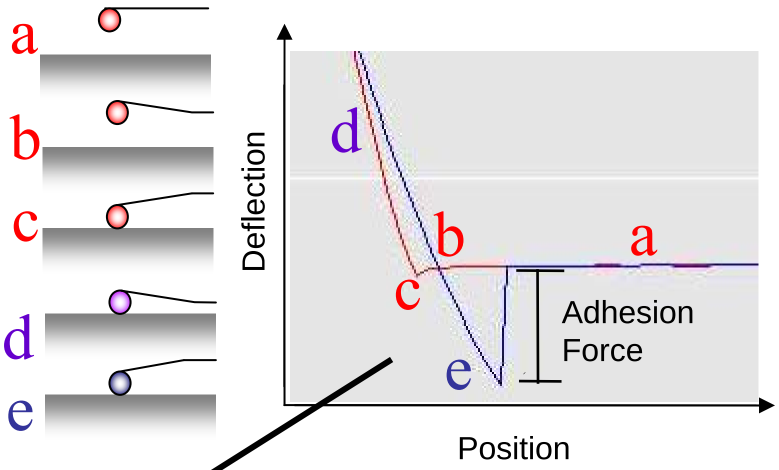
Al_2O_3 Particle

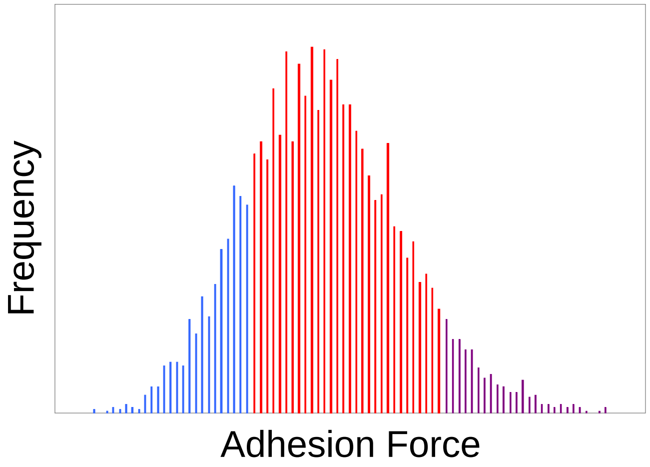


PSL Particle

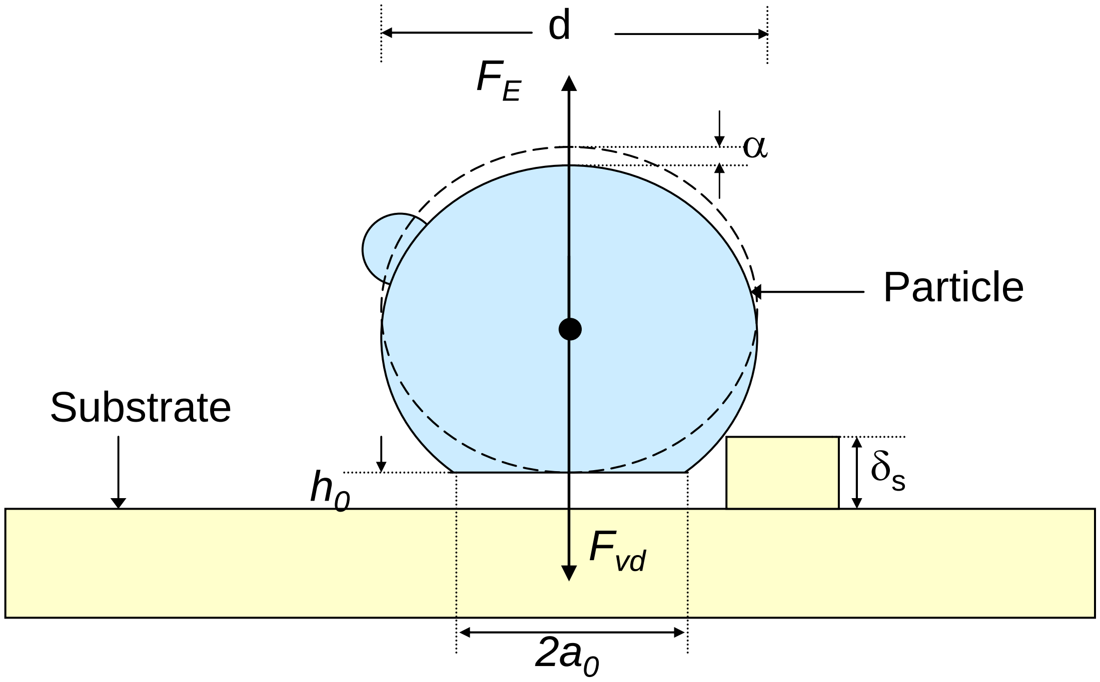


AFM Force Curve





The Model System



F_E = EDL Force

F_{vd} = VDW force

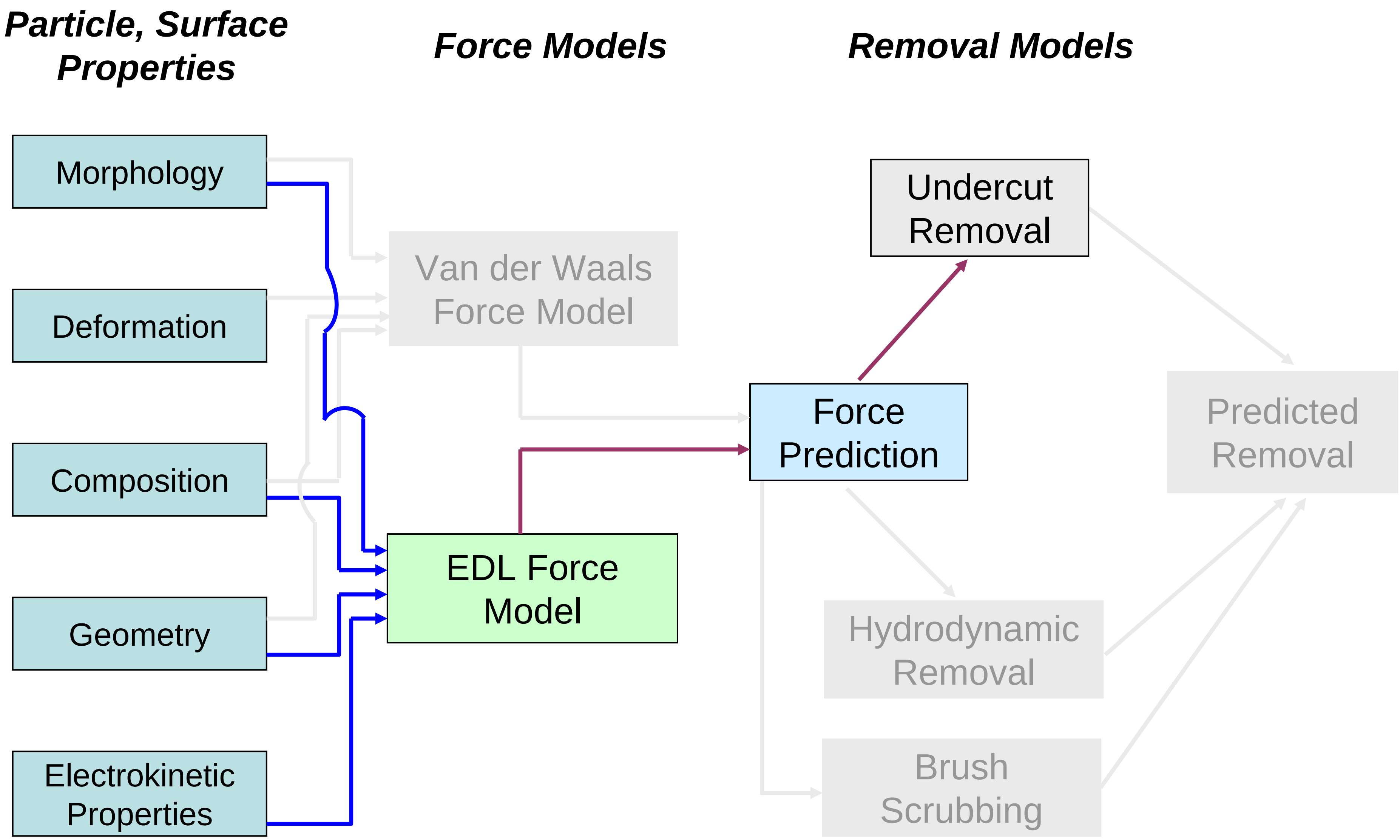
a_o = Contact radius

h_0 = 0.4 nm

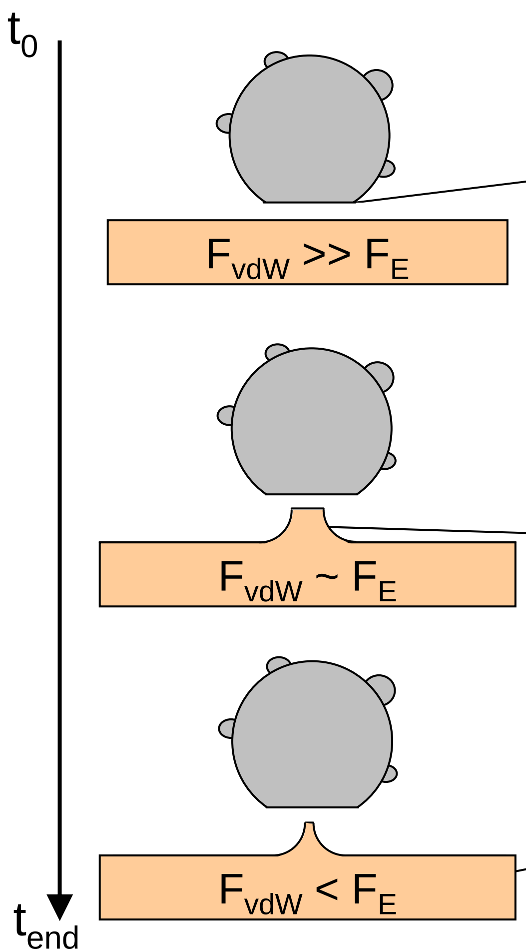
d = Particle diameter

- Rough, deformable spherical particle on a rough surface
- Particle deforms elastically – circular region of contact
- Particle is assumed to have attained equilibrium deformation

The Undercut Removal Model



The Undercut Removal Model



Particle undergoes elastic deformation → Contact radius (a)

$$a = \left[\frac{Ad^2}{4E^*h^2}\right]^{\frac{1}{3}}$$

$$E^* = \left[\frac{1-\upsilon_p^2}{E_p} + \frac{1-\upsilon_s^2}{E_s}\right]^{-1}$$

Undercut – due to isotropic wet etching → Etch rate model

Removal criterion using force balance → Two competing forces

- van der Waals force (F_{vdW})
- Electrostatic double layer force (F_{EDL})

Electrostatic Double Layer Force

$$F_E = \frac{\varepsilon\varepsilon_0 d\left(\psi_p^2+\psi_s^2\right)}{4}\cdot\frac{\kappa e^{-\kappa h}}{1-e^{-2\kappa h}}\cdot\left[\frac{2\psi_p\psi_s}{\psi_p^2+\psi_s^2}-e^{-\kappa h}\right]$$

$$F_{E,total}\Big|_t = F_{E,deform}\Big|_t + \int_a^b F_E\left(h(x)\big|_t\right)dx$$

d = Particle diameter

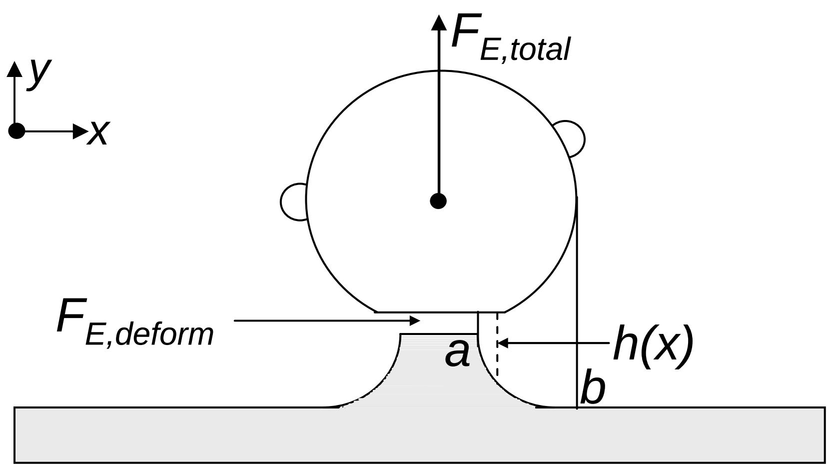
h = Particle-surface separation distance

ε = Medium dielectric constant

ψ = Zeta potential (*f(I,pH)*)

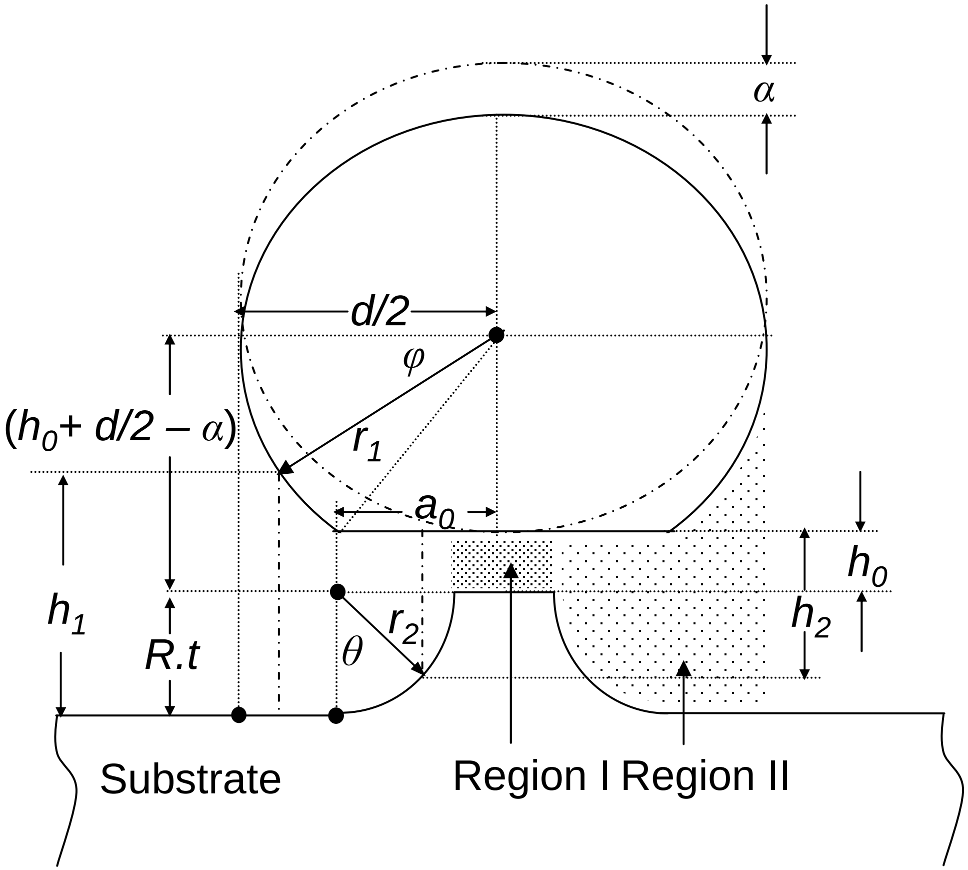
κ = Reciprocal double-layer thickness

I = Medium ionic strength



- Electrostatic double layer (EDL) force
  - *can be attractive or repulsive*
- EDL Force is a function of:
  - *particle-surface separation distance*
  - *system Chemistry*
  - *particle, surface zeta potentials*

Geometry of the System



$$r_1 = \frac{d}{2}$$

$$r_2 = R \cdot t$$

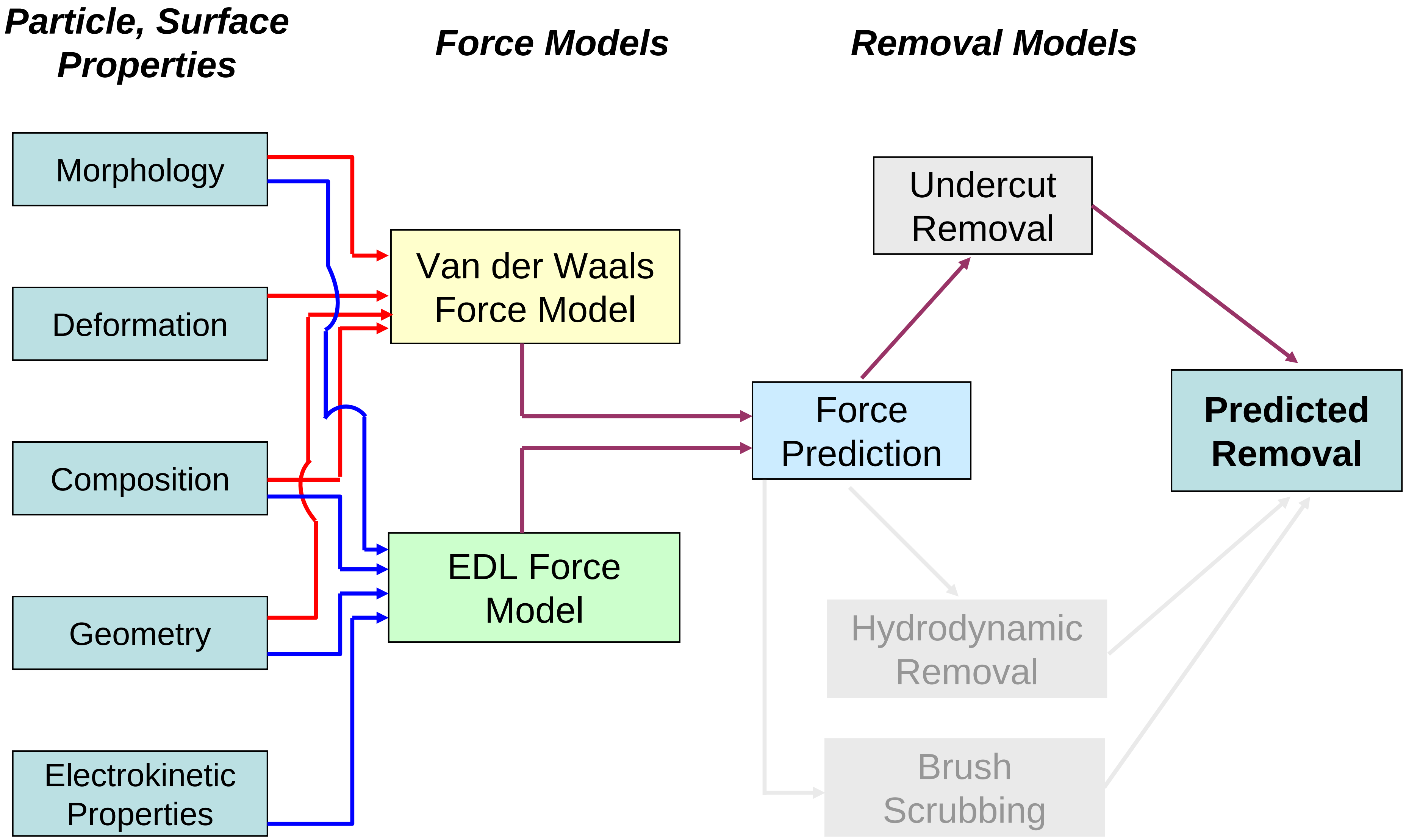
$$0 \le \varphi \le \left[\frac{\pi}{2} - \sin^{-1}\left(\frac{2a_0}{d} \right) \right]$$

$$0 \le \theta \le \frac{\pi}{2}$$

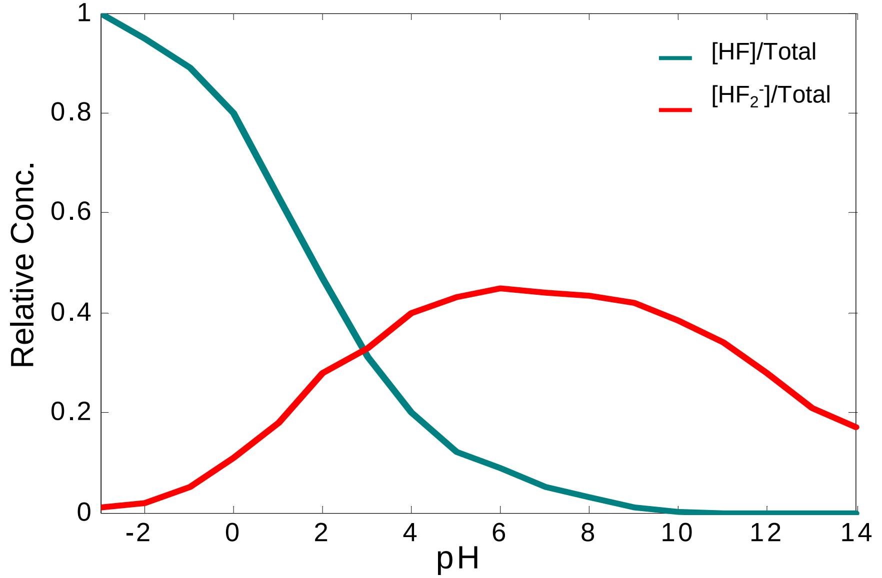
$$h_1 = h_0 - \alpha + Rt + \frac{d}{2}(1 - \sin\varphi)$$

$$h_2 = h_0 + Rt \sin\left(\frac{\pi}{2} - \theta \right)$$

Undercut Removal



Determination of Etch Rate (SiO_2 in 20:1 BHF)



System Kinetics*

$$K_1[HF] = [H^+][F^-]$$

$$K_2[HF_2^-] = [HF][F^-]$$

$$K_1 = 1.3 \times 10^{-3}$$

$$K_2 = 0.104$$

$$A = 2.5 \quad B = 9.66 \quad C = -0.14$$

$$Etch\ Rate = A[HF] + B[HF_2^-] + C$$

* Monk et al. Thin Solid Films, **232**, 1 (1993)

Particle Removal by Undercut Etching

- Etch rate of TEOS-sourced silicon dioxide in 20:1 BHF = ***R* = 31nm/min**
- Etching was carried out in excess of BHF – no mass transport limitations
- Undercut etching results in –

  - Decrease in contact area (deformed region)

$$a(t) = a_0 - Rt$$

a(t) = instantaneous contact area
a_0 = equilibrium contact area

  - Increase in particle – surface separation distance

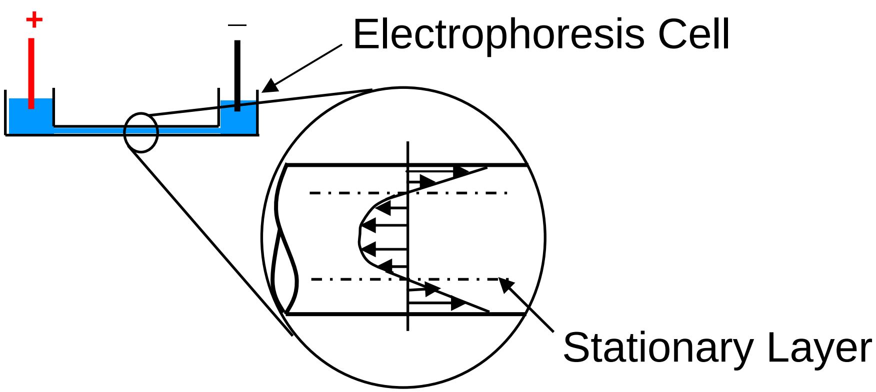
$$h(t) = h_0 + Rt$$

h(t) = instantaneous separation distance
h_0 = initial separation distance

- Removal occurs at a given *a(t)* and *h(t)* for which $F_{vdW} < F_E$

Measurement of Electrokinetic Potentials

Particle Zeta Potentials



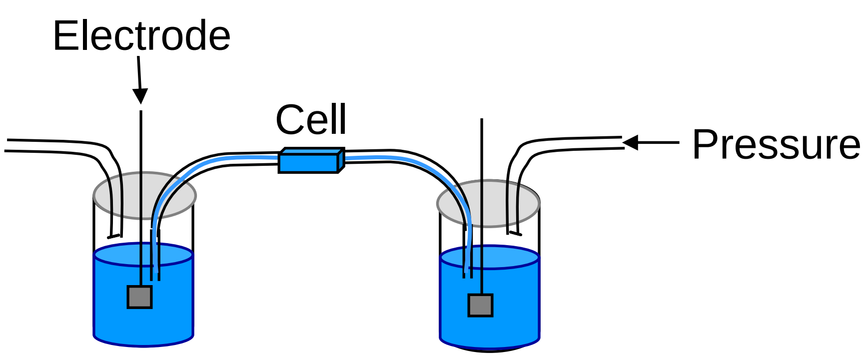
Smoluchowski Equation

$$\zeta = 113{,}000 \frac{\mu}{\varepsilon} \text{EM} \quad (\text{mV})$$

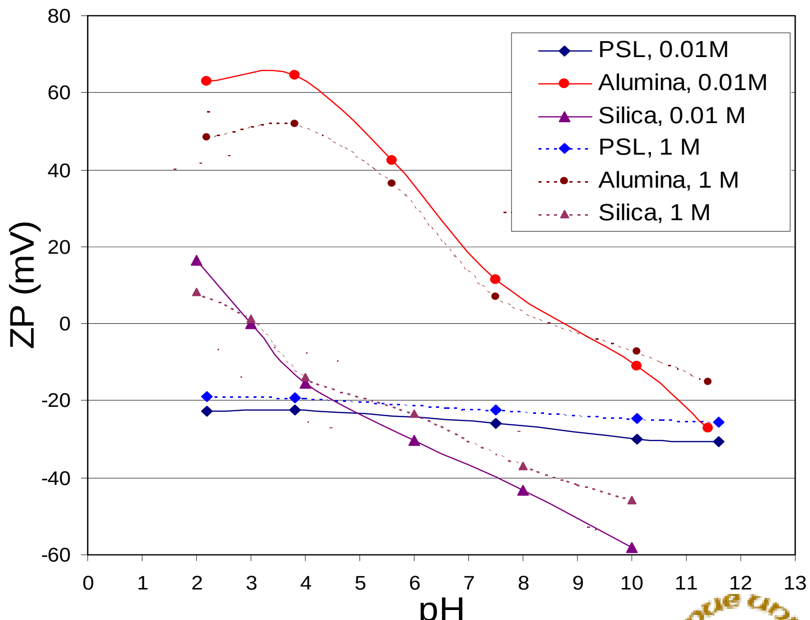
Streaming Potential Equation

$$\zeta = 135500 \frac{\Phi \mu k_e}{\Delta P \varepsilon \varepsilon_o} \quad (\text{mV})$$

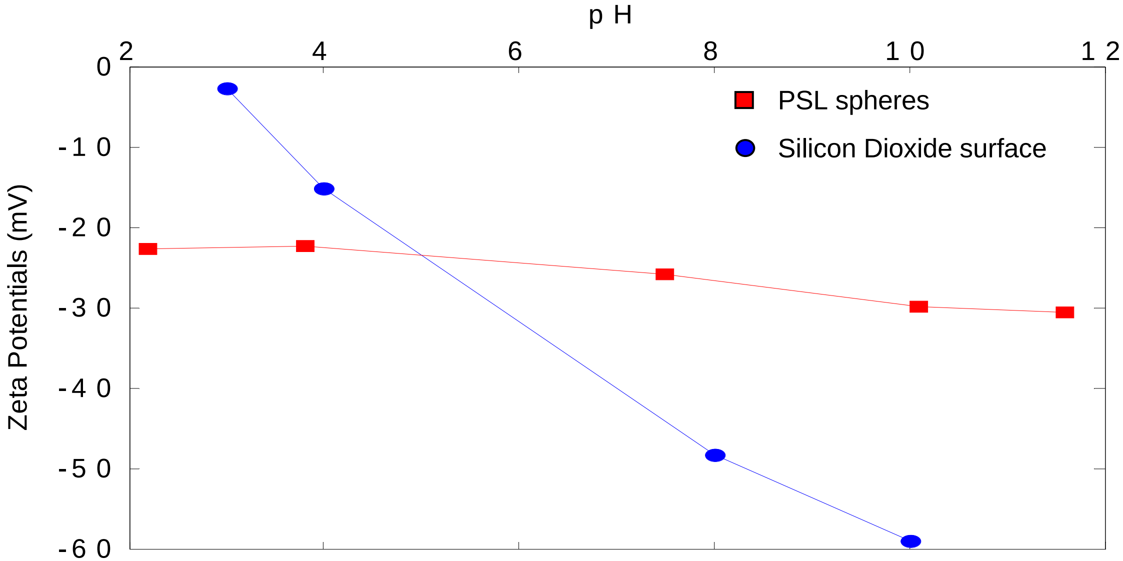
Surface Streaming Potentials



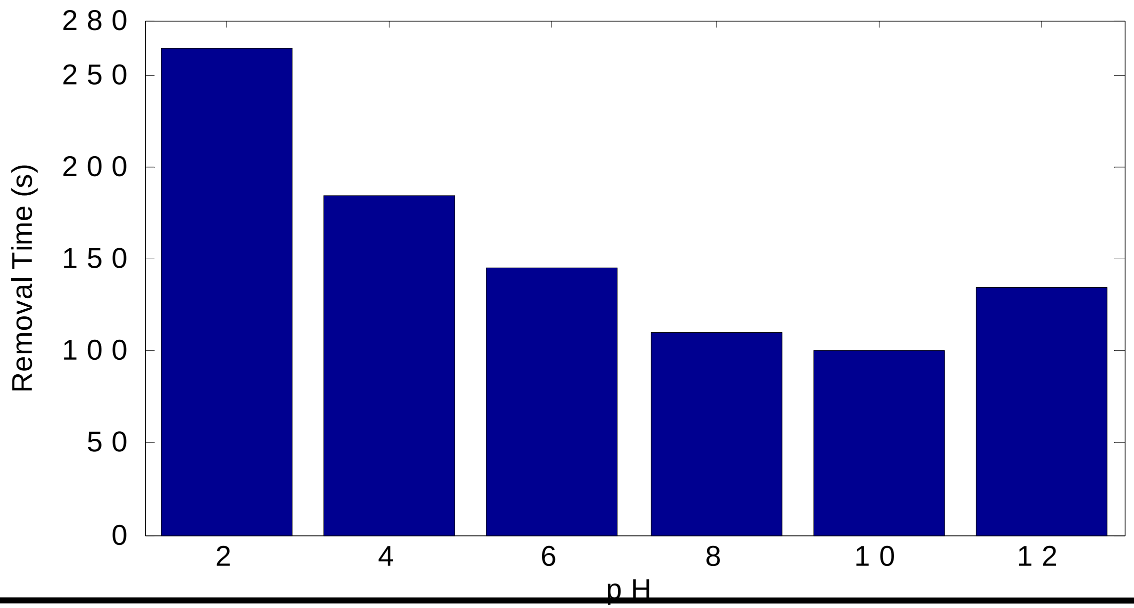
Potentials as a function of pH



Dependence of Removal on pH

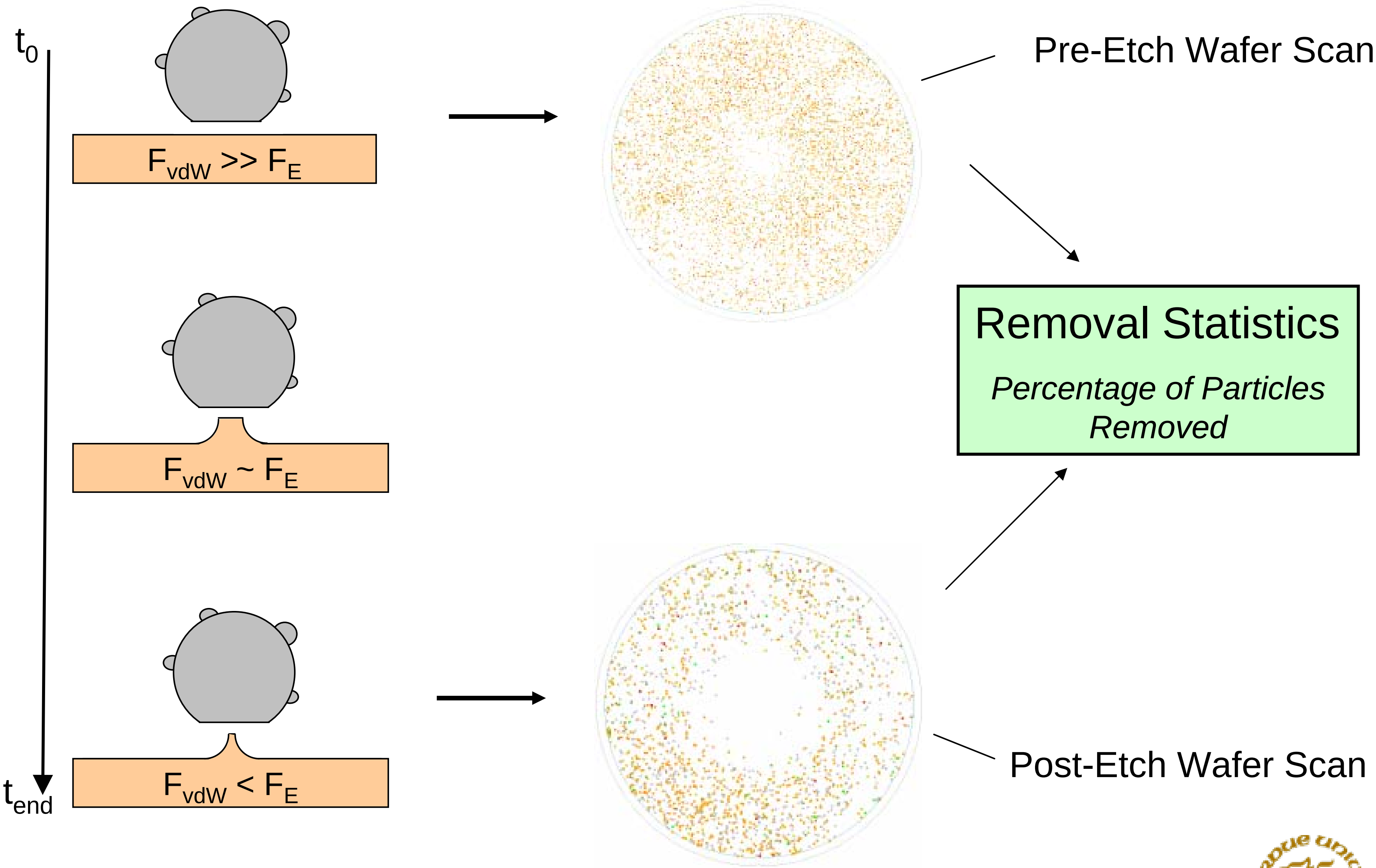


Zeta potentials were measured for a 1:1 electrolyte system



Predicted removal time for 15 µm PSL spheres on TEOS-sourced silicon dioxide surface

Removal Experiments



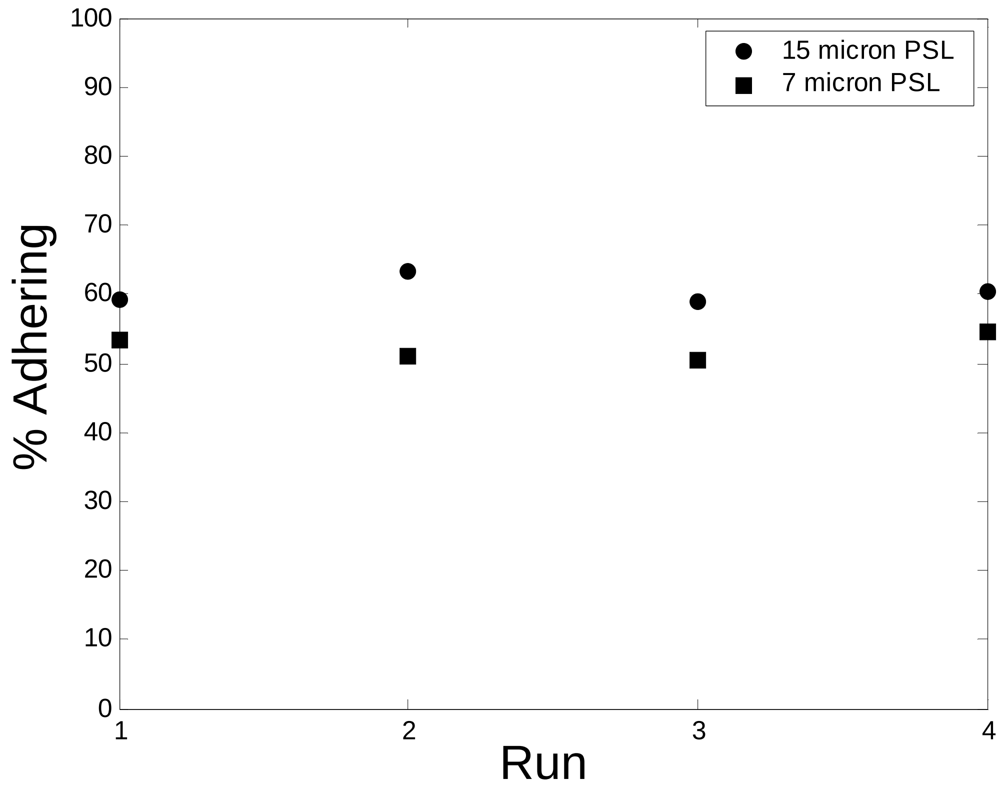
Experimental Procedure

- 7 and 15 µm PSL spheres were spray deposited onto 200mm wafers with TEOS-sourced SiO_2
- Particles were allowed to settle for 24 hrs on the surface to allow them to deform
- Pre-Etch scan of the wafer surface was obtained using a Tencor Surfscan SP1 system at SEZ, America
- The wafers were immersed in 20:1 BHF solution at 25 ^{o}C for various etch times. The etch bath was stagnant to avoid particle removal due to hydrodynamic forces
- Post-Etch scans were obtained using the Surfscan system and the percentage of particles adhering was determined

Effect of Immersion and Short Etch Time

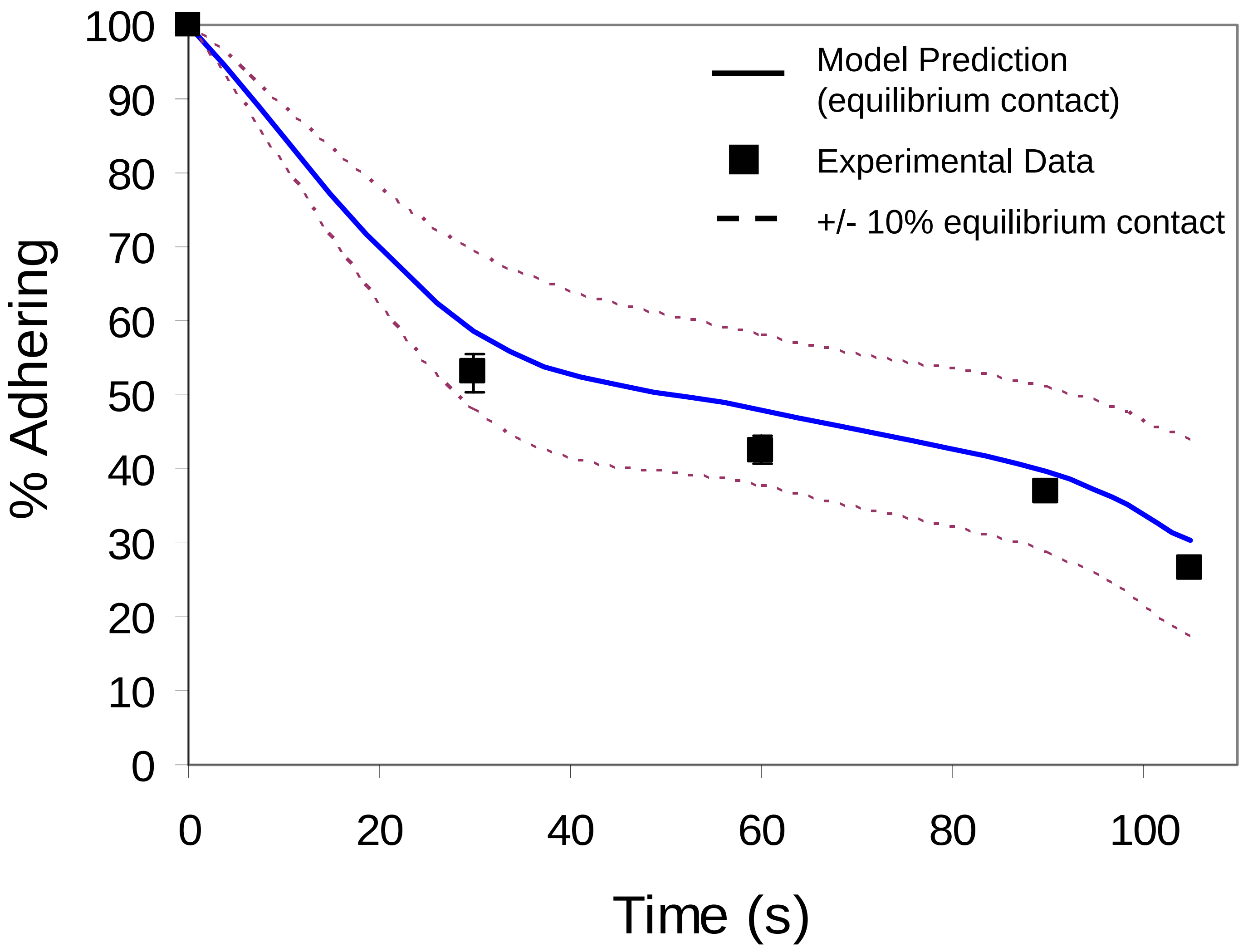
Particle Size	Fraction particles adhering	Deviation
7 µm	0.91	± 0.01
15 µm	0.95	± 0.03

Effect of immersion on particles adhering

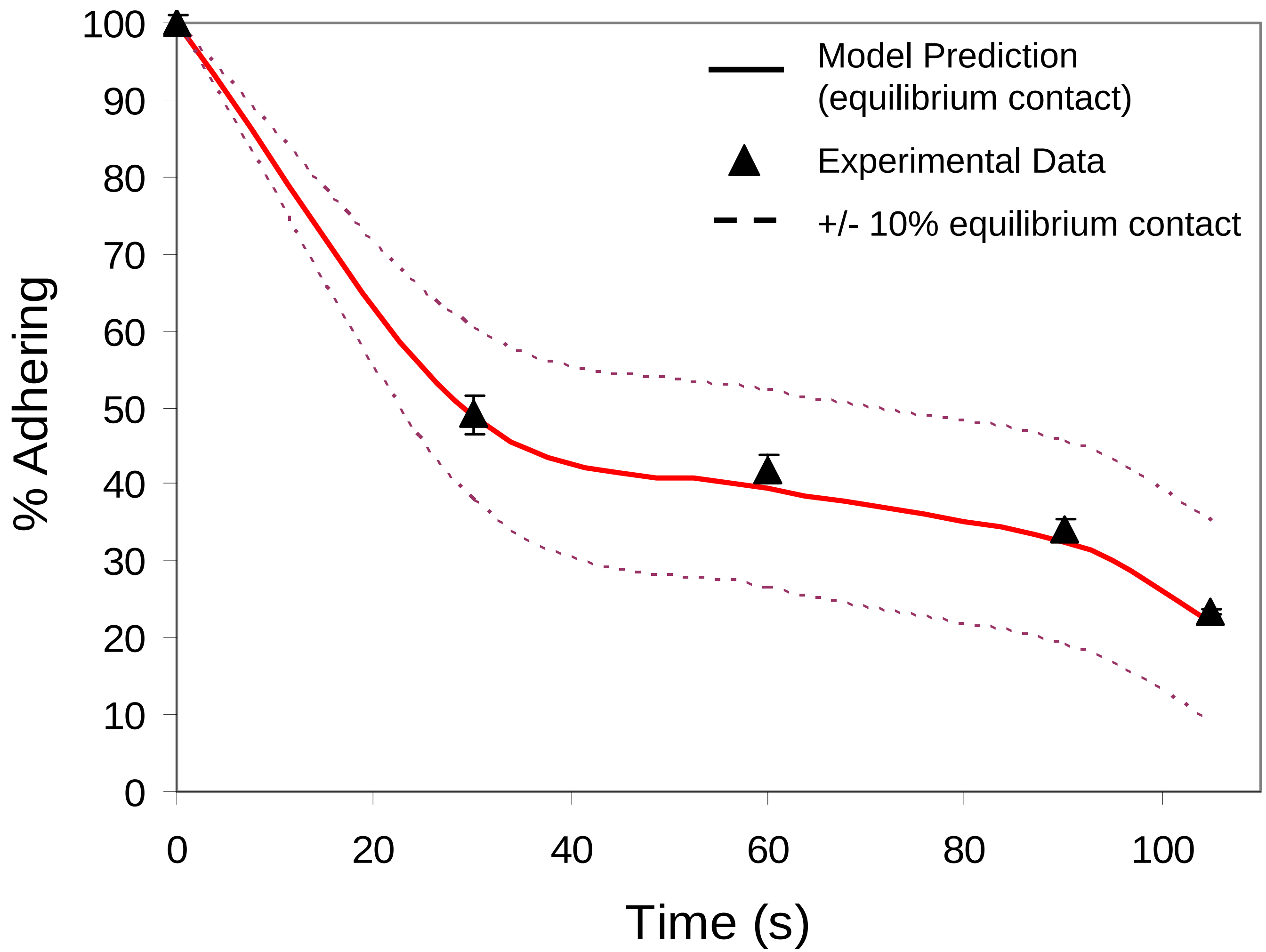


Effect of 10 s etch on particles adhering

Model Validation (15 µm PSL)



Model Validation (7 µm PSL)



Conclusions

- Particle removal highly dependent on adhesion through
  - Particle size distribution
  - Roughness
- Zeta potentials of the particle and surface play an important role in determining ease of particle removal
- Undercutting results in increased particle-surface separation distance and decreased particle-surface contact area
  - Results in reduction of net adhesion force
- Predictions from the undercut removal model agree well with experimental data

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