Particle Adhesion and Removal in Semiconductor Processing

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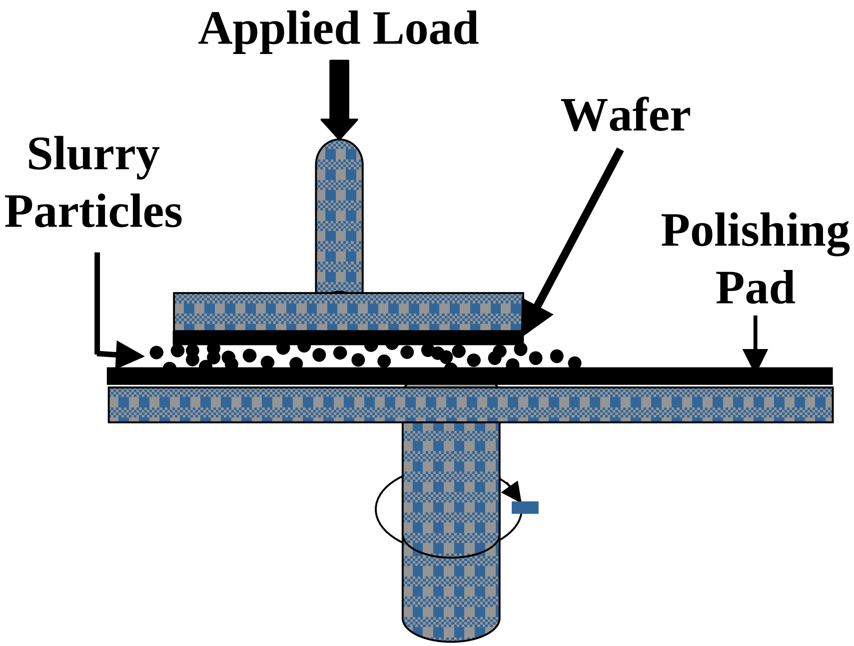
Chemical Mechanical Polishing (CMP)



CMP Tool

- Removes a thin surface layer to obtain planarity of wafers
  - Uses abrasive particles in aqueous solution in conjunction with relative motion between polishing pad and wafer
  - Surface removed mechanically and chemically
- Introduces contaminants onto wafer surfaces
  - Pieces of polished surface and polishing pad
  - Slurry particles
  - Contamination from the handler or handling device
  - Must be removed before further processing

Post-CMP Cleaning

» Must remove particles less than 1 micron in diameter

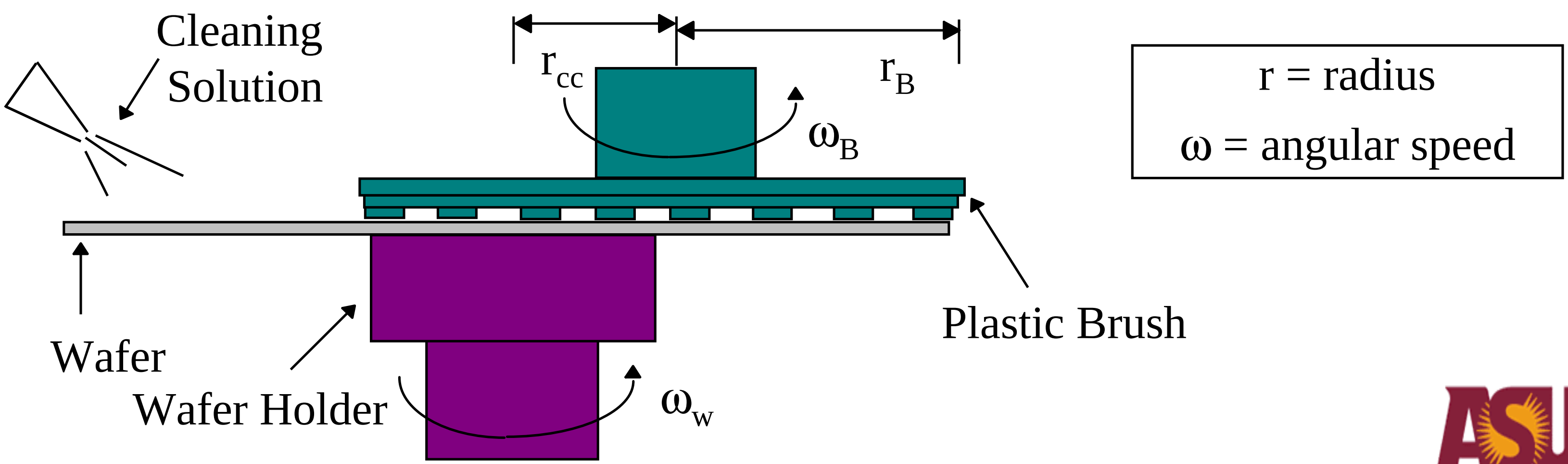
» Must not roughen wafer surface excessively

» Brush scrubbing and megasonic cleaning have potential for removing small particles

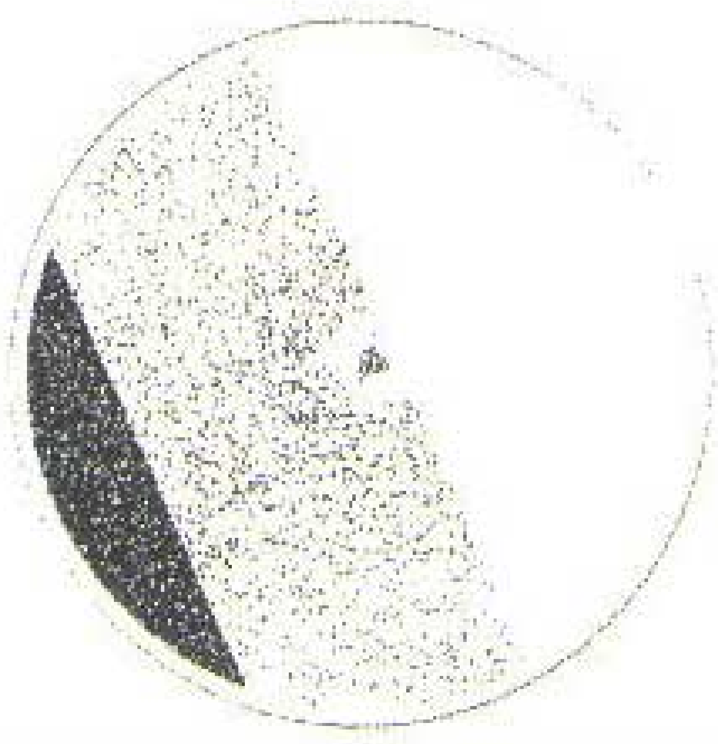
» Problems with

- Resource consumption
- Lack of understanding of cleaning mechanism
- Inefficient and unreliable processes

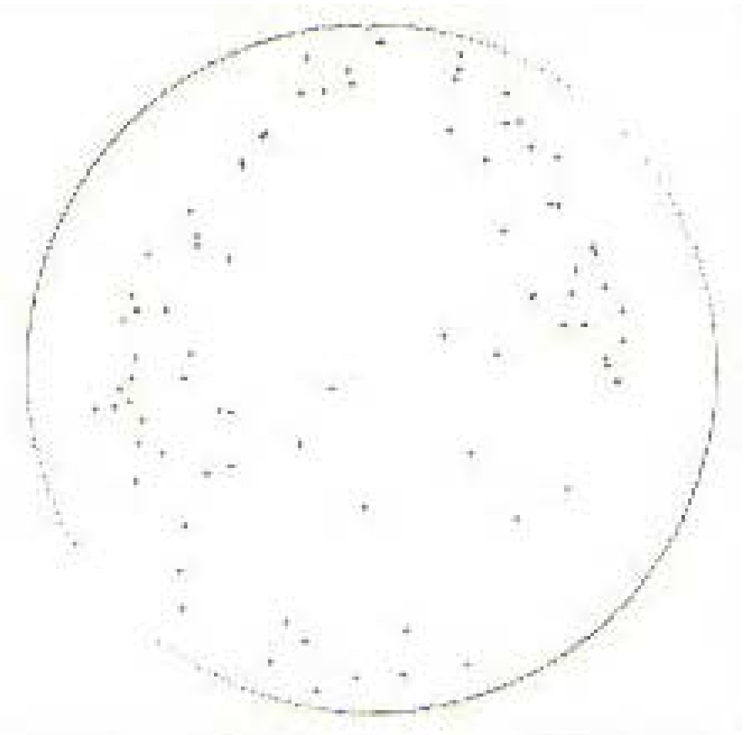
Brush Scrubber



Brush Scrubbing Results[†]



Before Cleaning



After Cleaning

[†]*Zhang, Burdick, and Beaudoin. Thin Solid Films 332, 379 (1998)*

Post-CMP Cleaning Model Objective

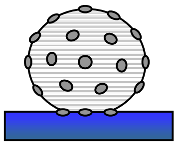
Develop and validate scientifically-based cleaning models to optimize wafer cleaning processes and minimize water and chemistry use

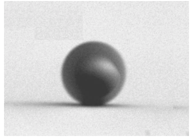
Adhesion Model

Removal Model

<u>1st Generation</u>

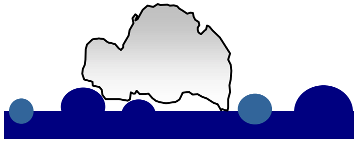
Rough deformable spherical particles interacting with a rough flat surface



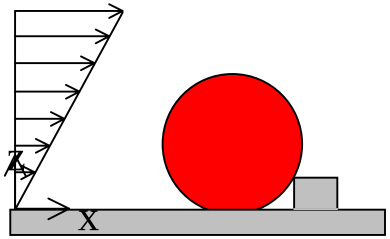


<u>2nd Generation</u>

Asymmetrical rough particles interacting with any surface



Use critical particle Reynolds approach to determine flow conditions needed to initiate particle removal

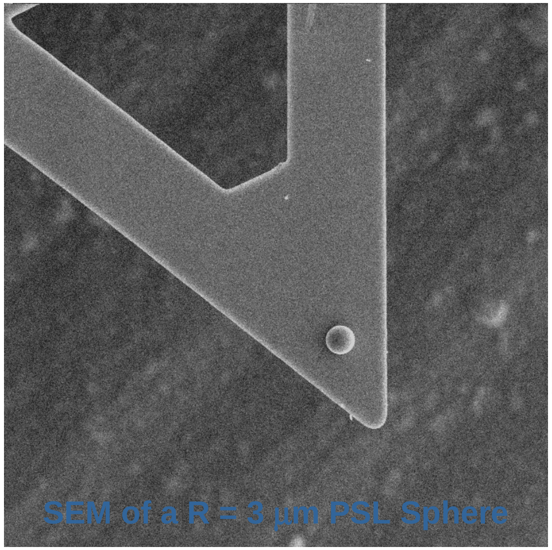


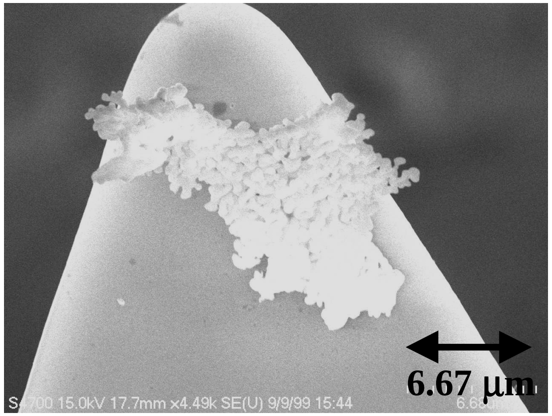
Adhesion Mechanisms

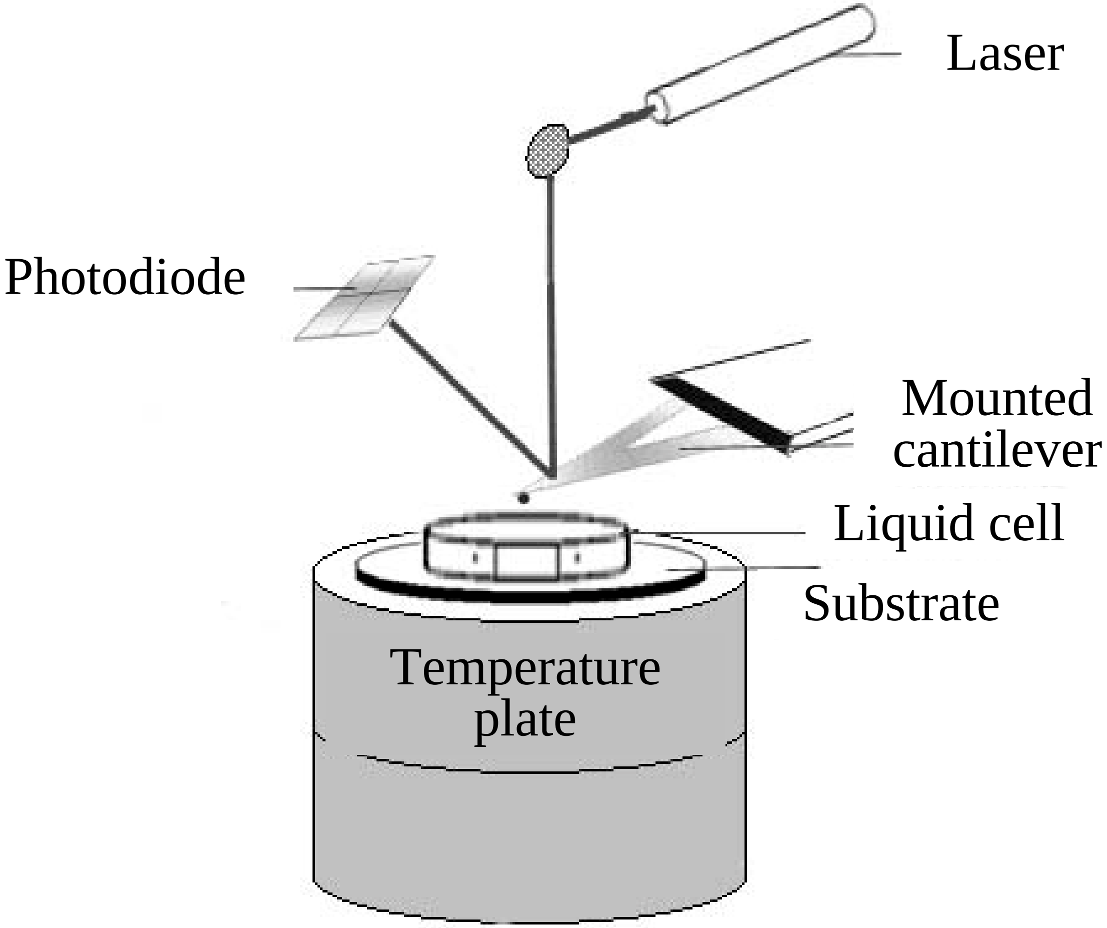
Bond Type	Interatomic Distance (Angstroms)	Dissociation Energy (Kcal/mole)	Effect of Temperature
Primary Covalent	1 to 2	50 to 200	None
H-H	0.8	104	
C-H	1.1	99	
C-C	1.5	83	
Ionic	2 to 3	10 to 20	High
Hydrogen Bond	2 to 3	3 to 7	High
van der Waals Forces			
Dipole Interactions	2 to 3	1.5 to 3	High
London Forces	**3 to 5**	**0.5 to 2**	**Low**

Always present

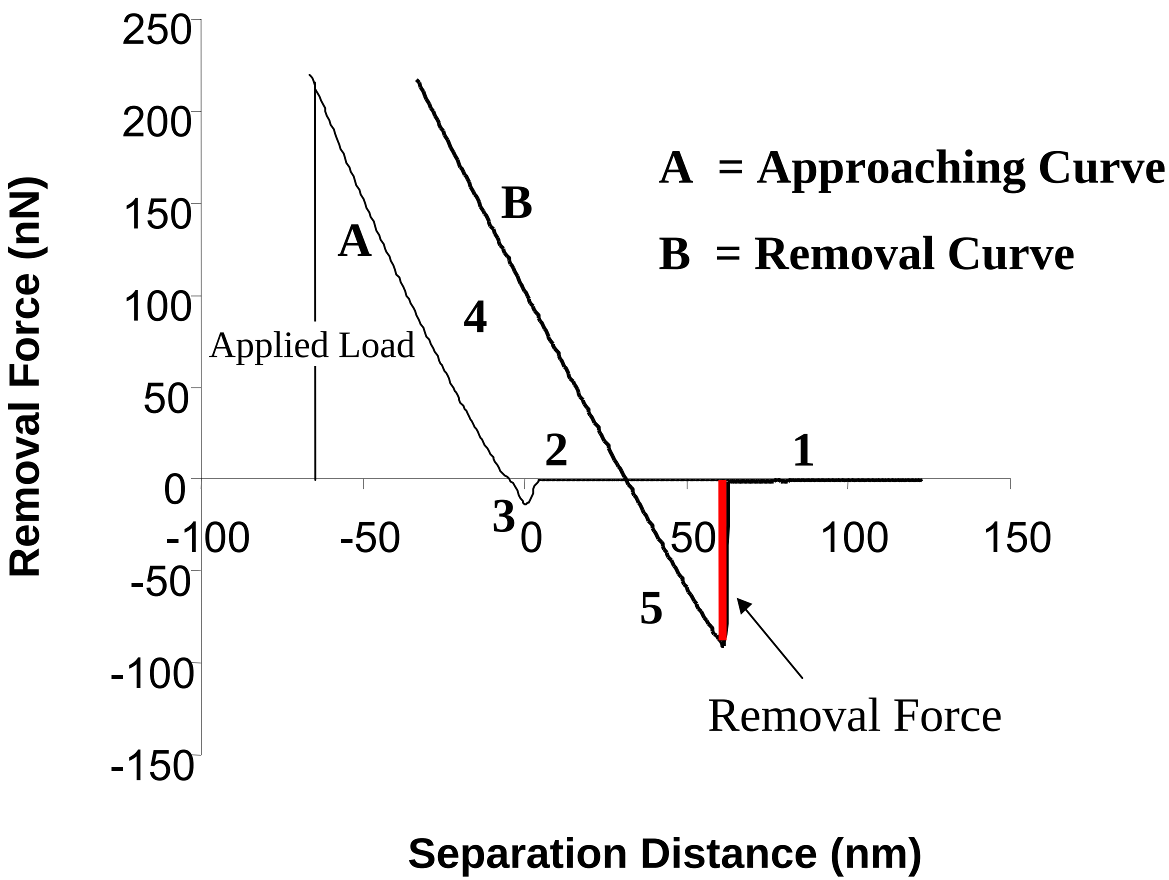
AFM Force Measurement

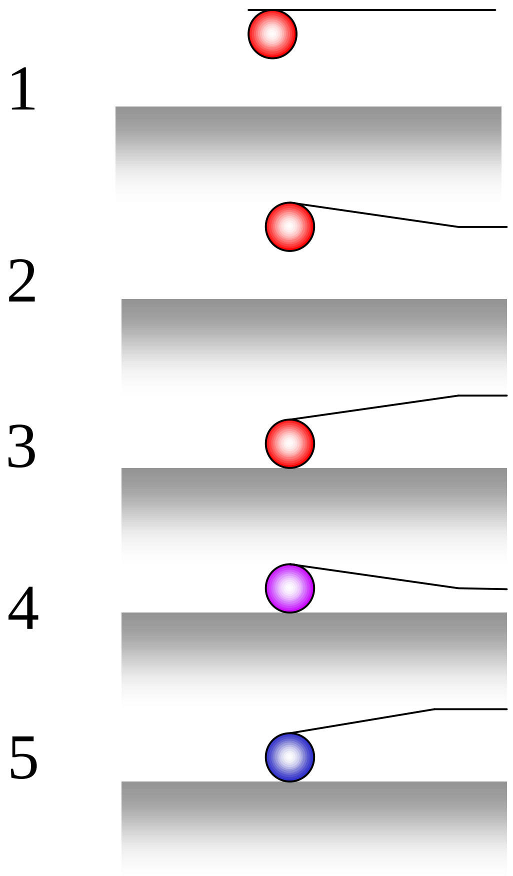




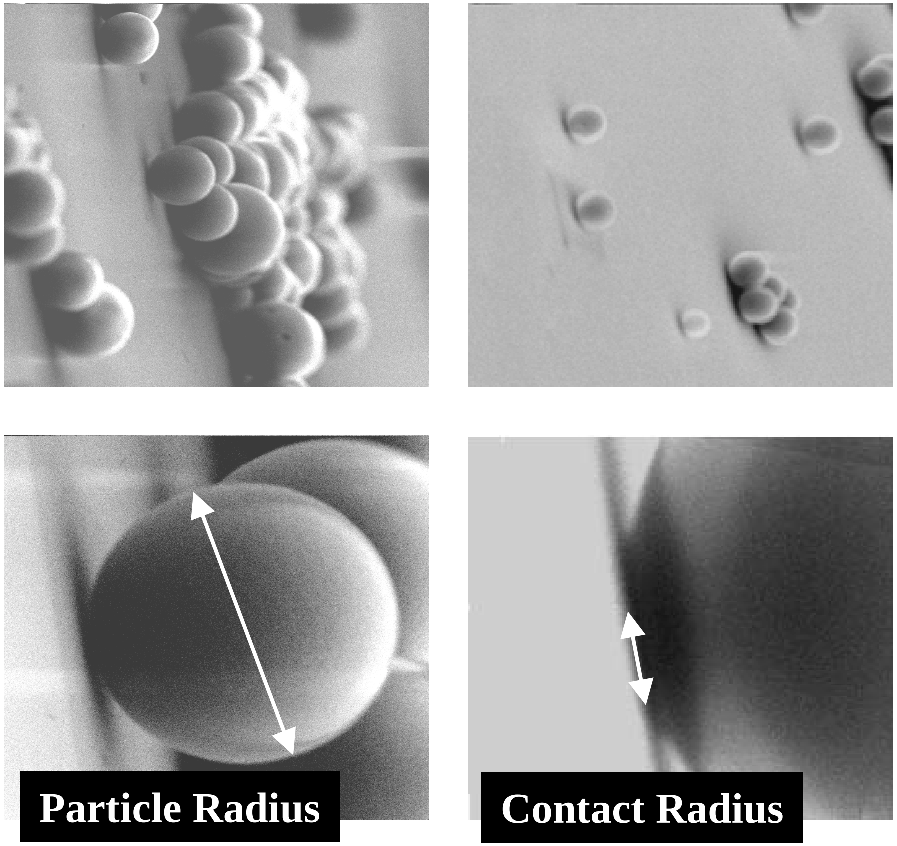


AFM Force Curve





Particle – Surface Contact Radius



PSL spheres on Silicon

Elastic-plastic deformation

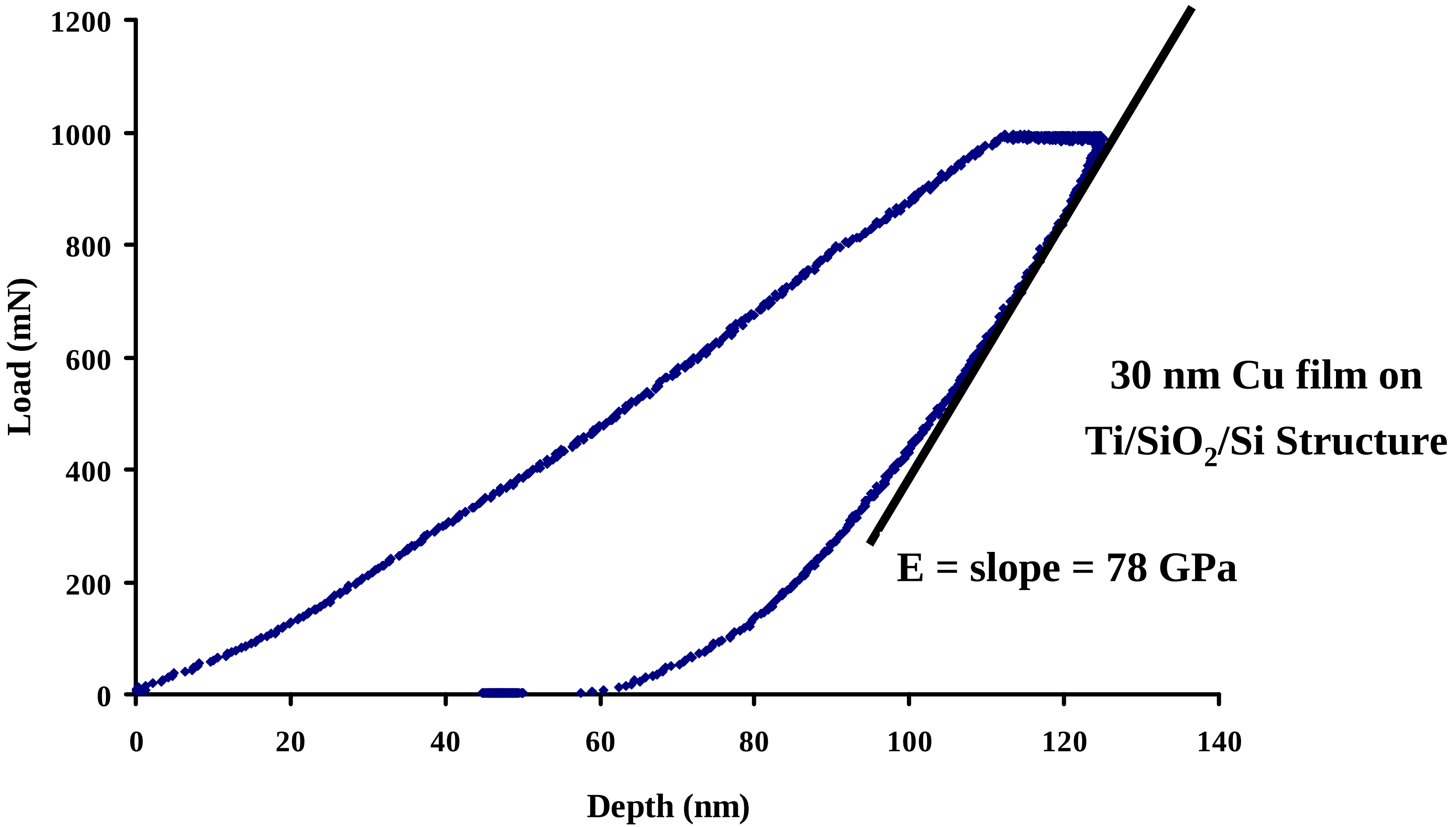
$$a = 0.43 \cdot R^{0.53}$$

Adhesion-induced contact radius (μm)

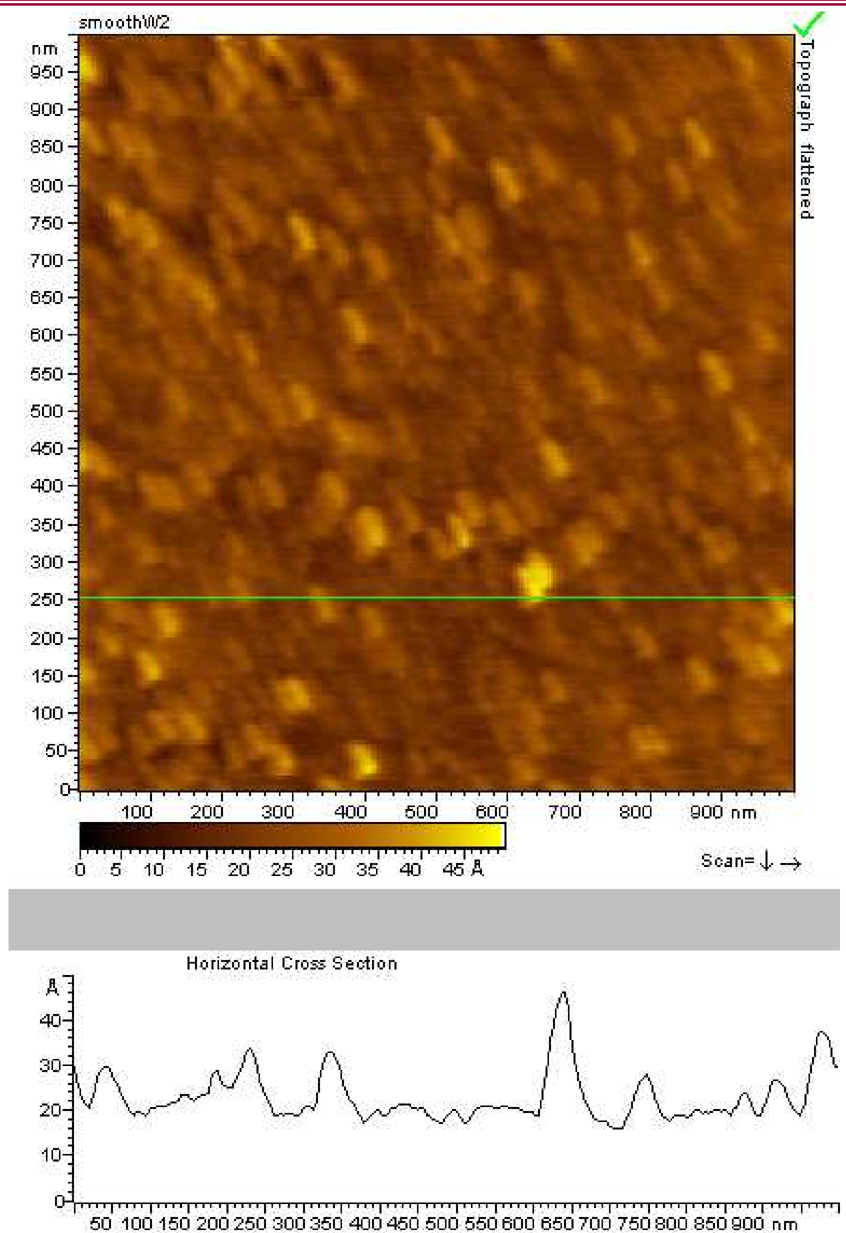
Particle radius (μm)

Surface Mechanical Properties

Force / Depth profile from a Hystem Nanoindentor



Particle and Surface Morphology



4 Parameters Determined

Average asperity size (ε_s)

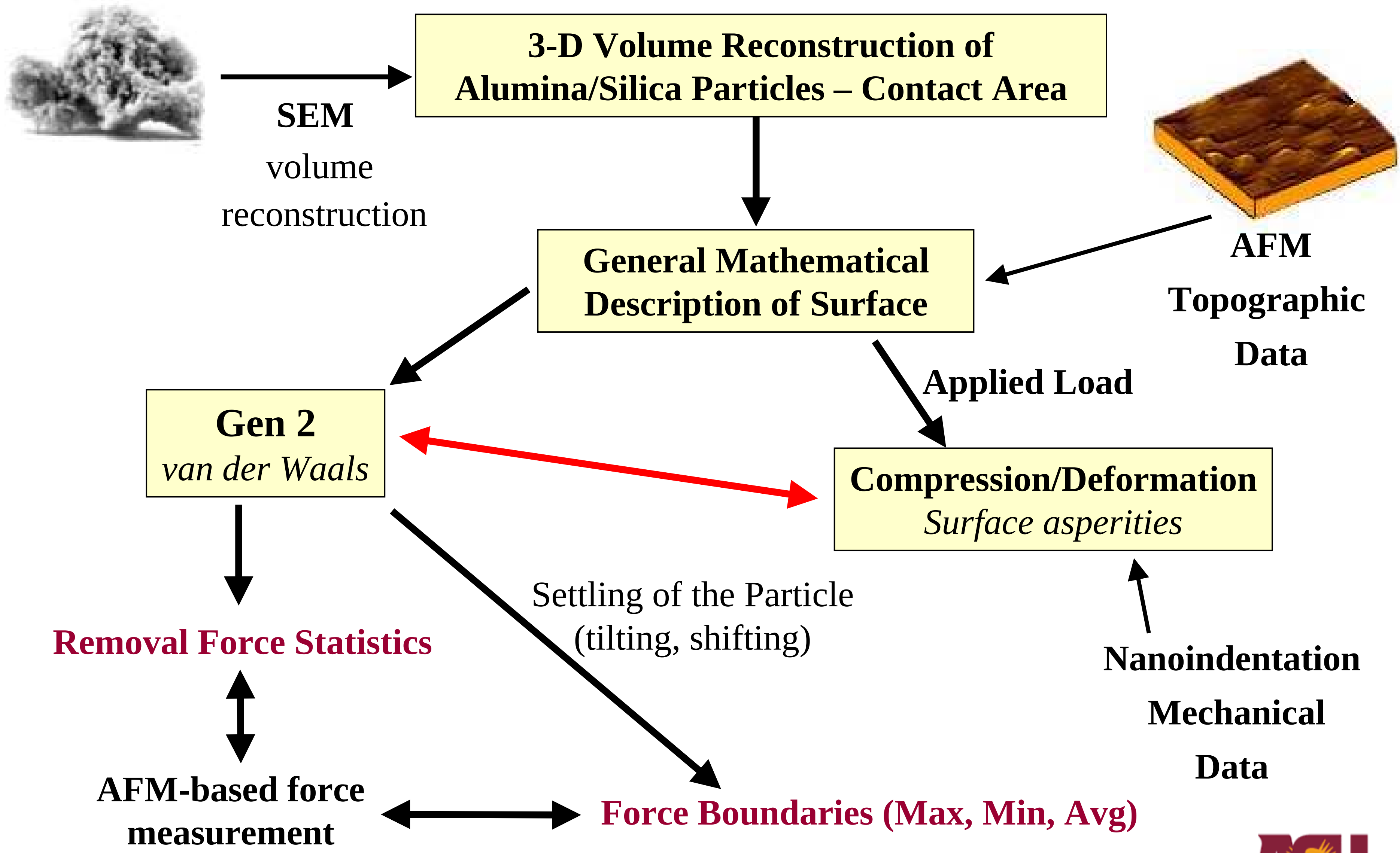
Standard deviation in asperity size (std)

Fractional coverage of the surface by asperities (f)

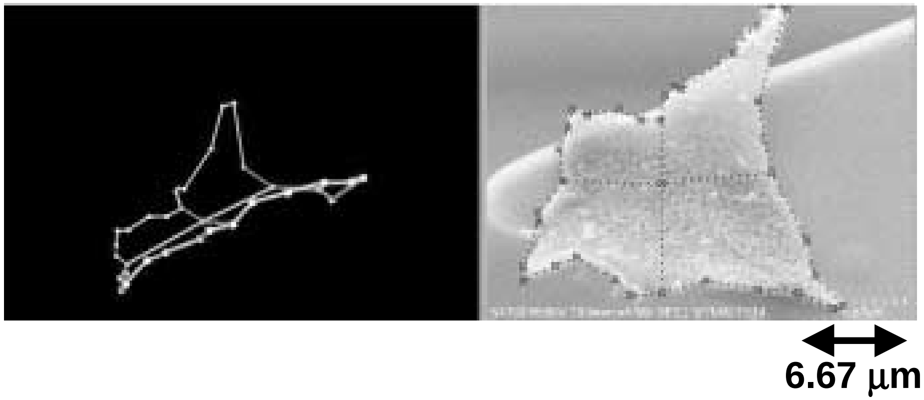
Common shape, if any, among asperities

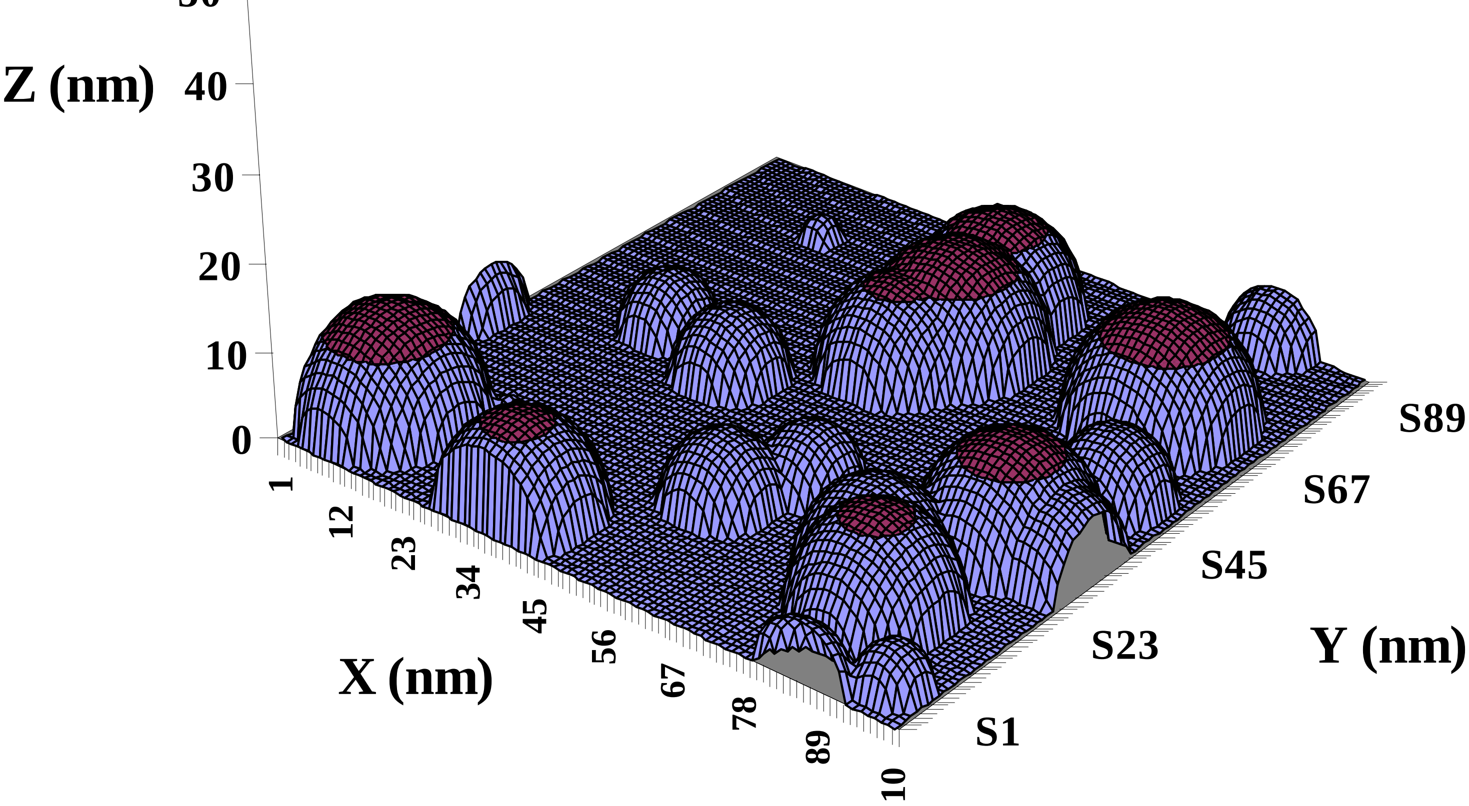
Asperities assumed to be hemispherical in this work

2nd Generation Model (Gen 2)

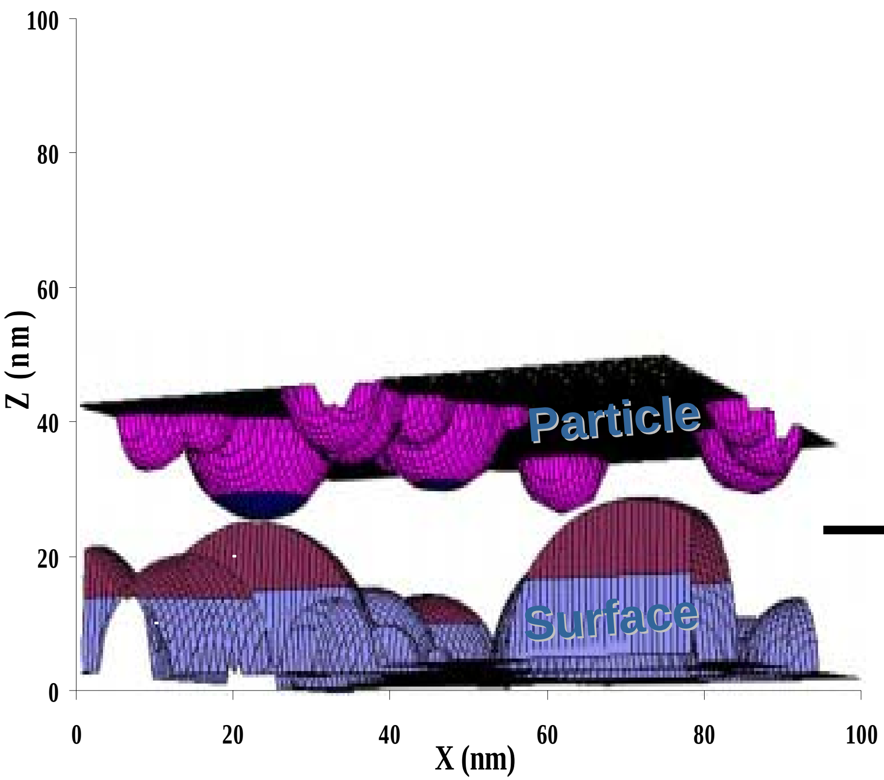


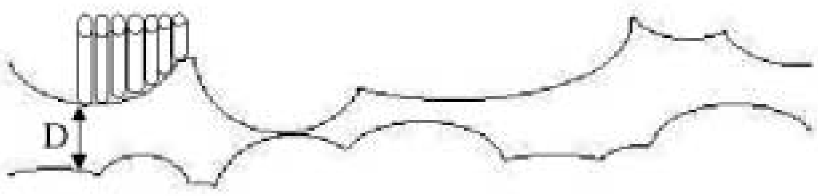
3-D Surface Reconstruction – Simulated Surface





Surface Interaction Force



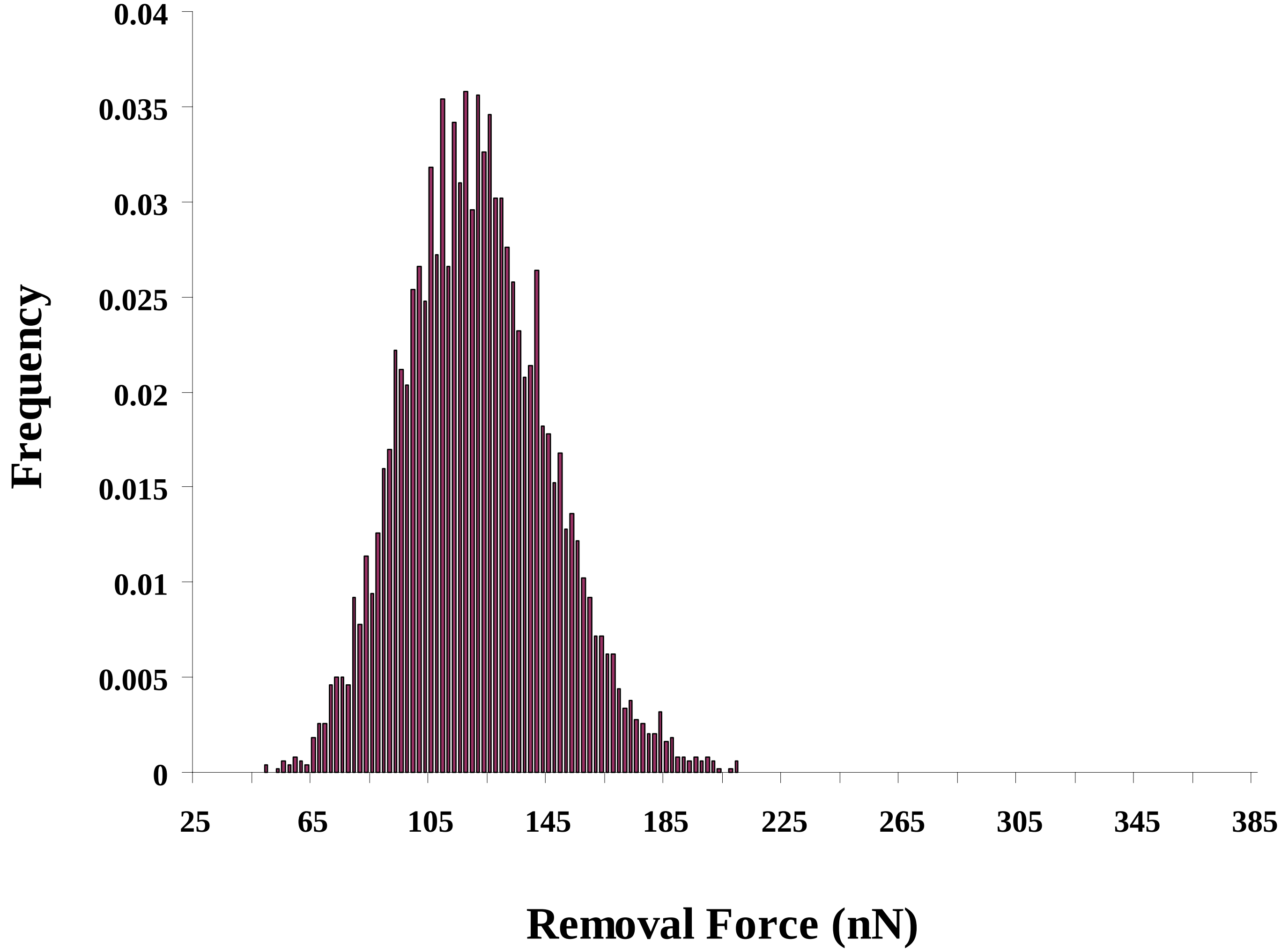


Cylindrical Volume Elements

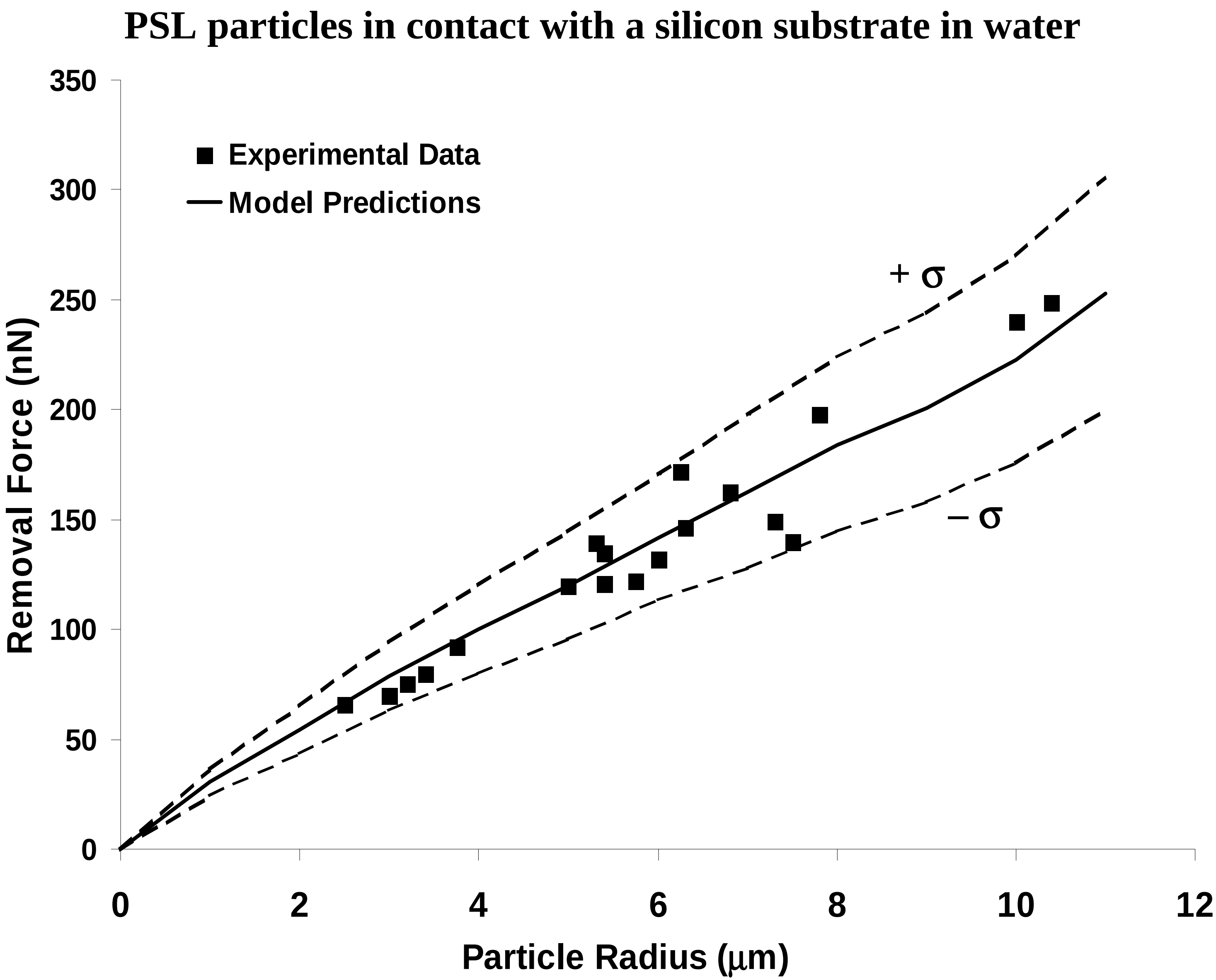
$$F_A = -\frac{A \cdot (\text{Area cylinder})}{6 \cdot \pi \cdot D^3}$$

Roughness Effect – Monodisperse Particles

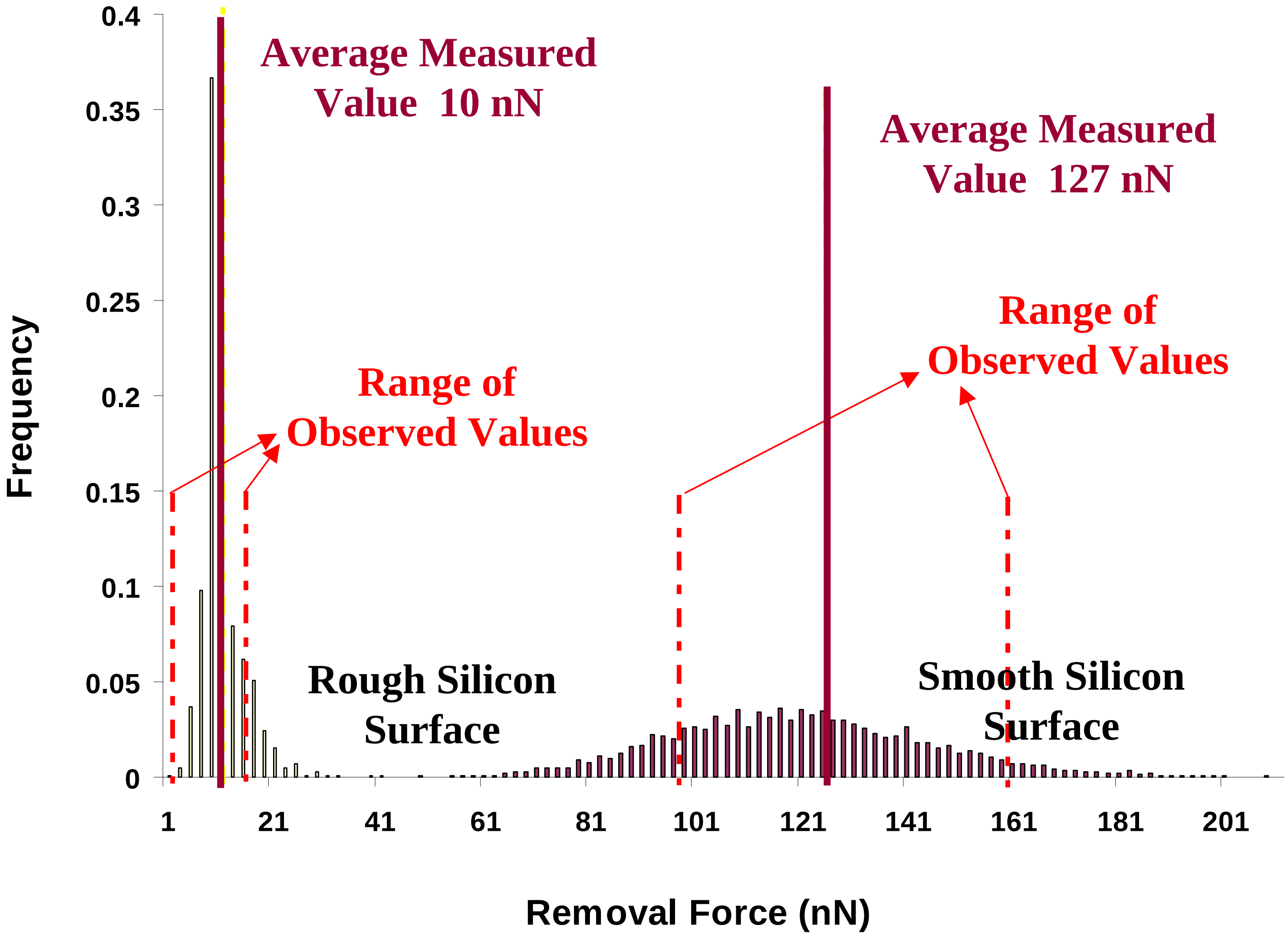
5 μm PSL in contact with a silicon substrate in DI water



Effect of Particle Diameter

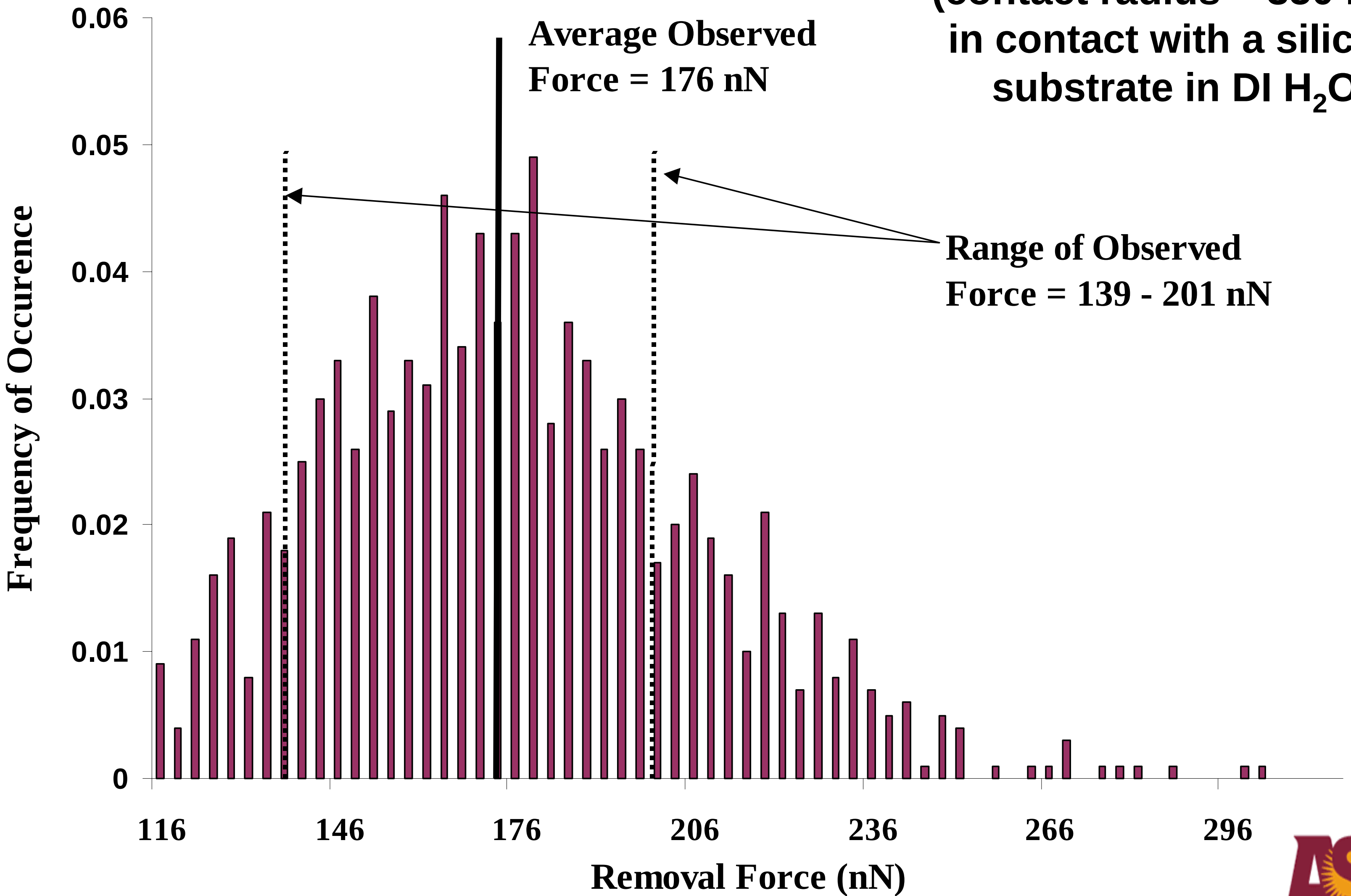


Validation of Substrate Roughness

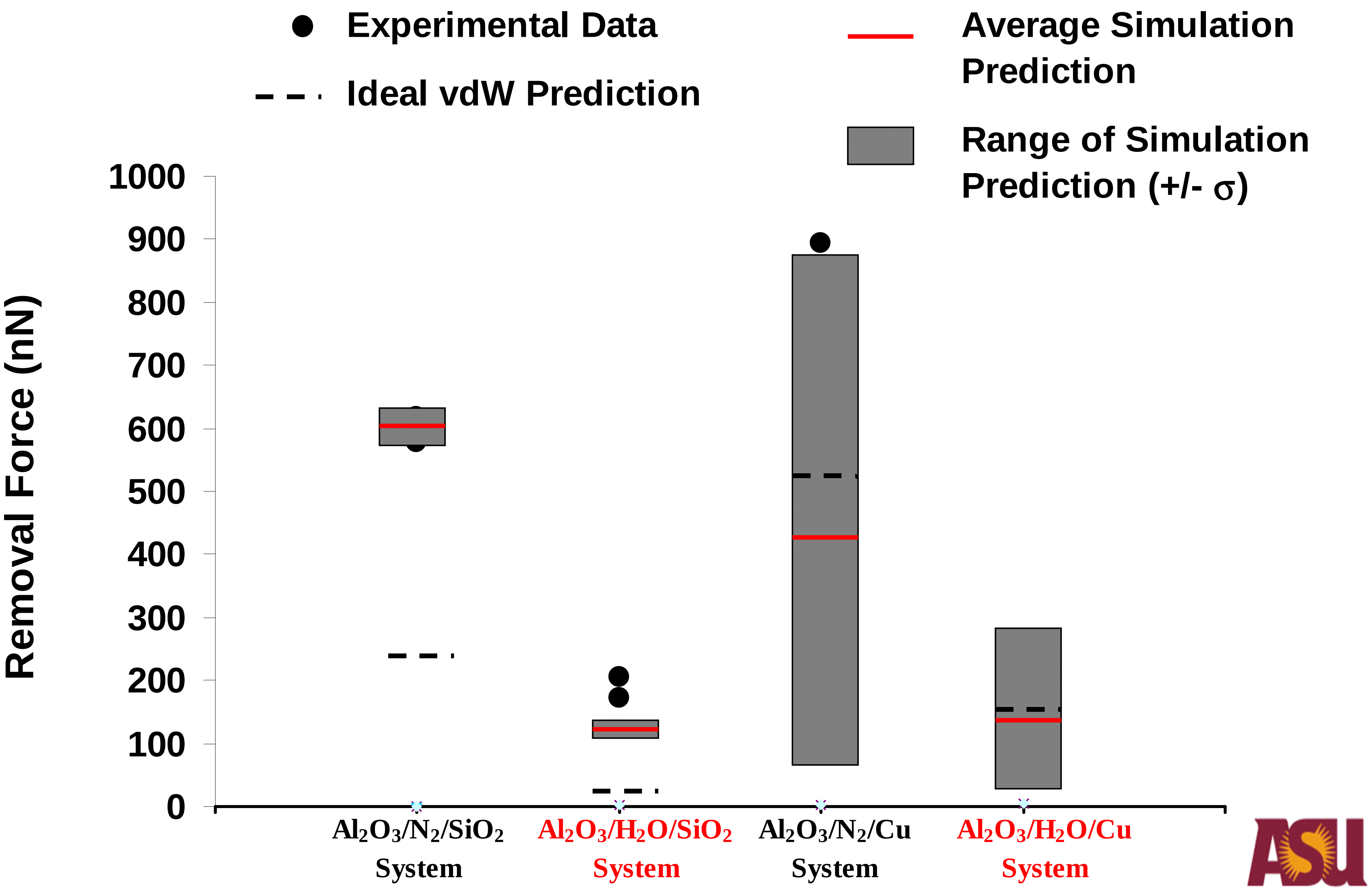


Alumina/H_2O/Silicon Adhesion

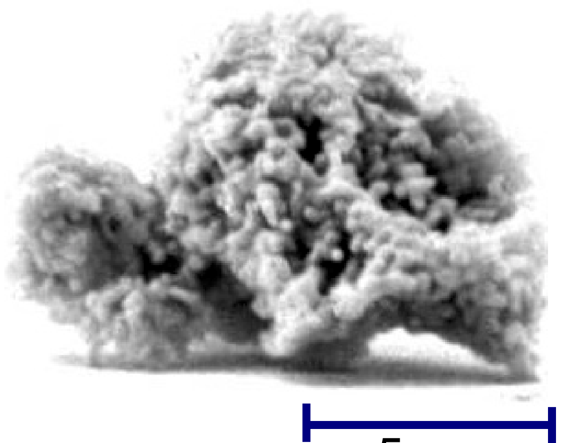
3 μm alumina particle (contact radius = 350 nm) in contact with a silicon substrate in DI H_2O

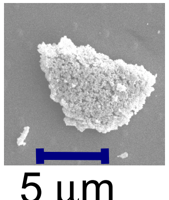


Alumina Adhesion – Effect of Substrate and Medium

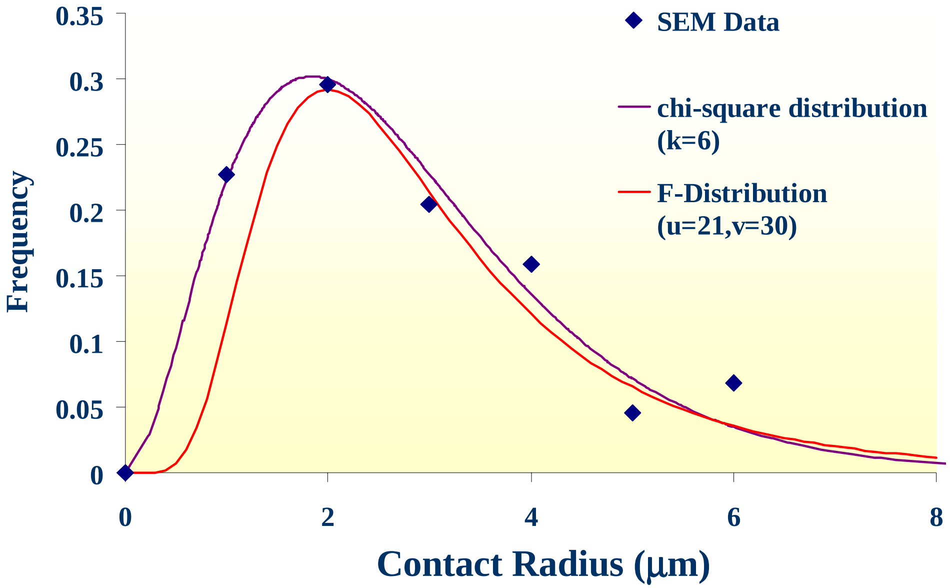


Geometry Effects





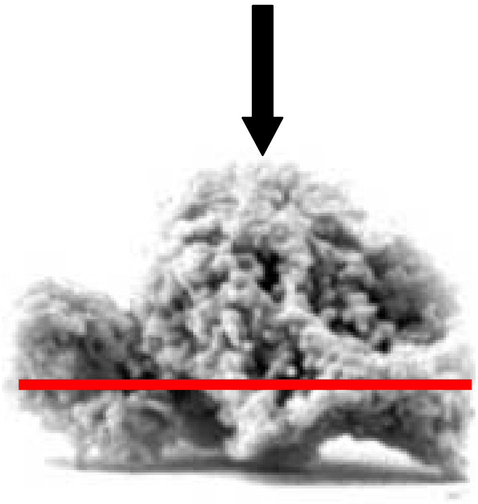
SEM of an alumina particle on a polished silicon substrate (15 KeV, 10000X, 87 degrees)



Current vdW models for a spherical 0.15 µm alumina particle (slurry particle) in contact with a silicon surface predict a removal force of 15 nN

Our simulation accounting for the larger than expected contact area predicts a removal force of 108 nN

Effect of Applied Load



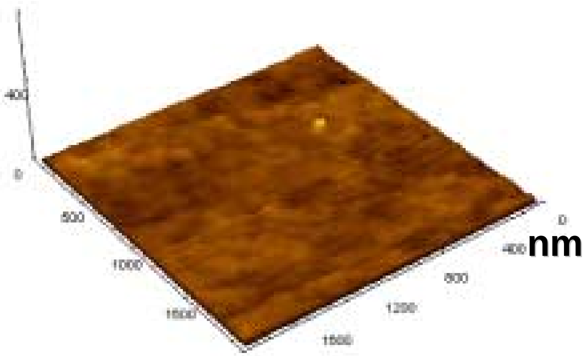
5 PSI Applied Load

Maximum contact area (0.15 μm alumina slurry = 282 nm)

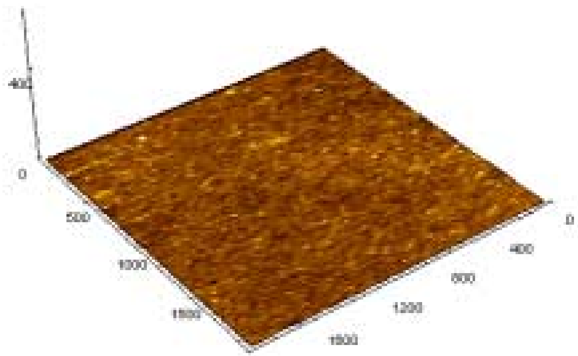
System	Force Prediction (nN) Applied Load = 0 PSI Smooth Films	Force Prediction (nN) Applied Load = 0 PSI Rough Films	Force Prediction (nN) Applied Load = 5 PSI Rough Films
Al_2O_3/Air/SiO_2	289	108	4058
Al_2O_3/Air/Cu	653	46.3	5876
Al_2O_3/Air/W	676	56.1	5335
Al_2O_3/H_2O/SiO_2	39.2	3.3	544
Al_2O_3/ H_2O/Cu	186	11.5	1674
Al_2O_3/ H_2O/W	200	16.6	1555

Post-CMP Cleaning – Surface Characterization

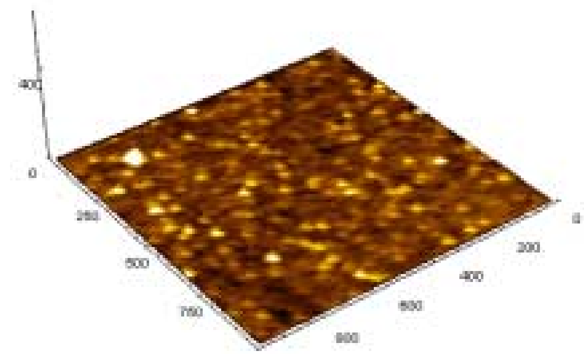
All axes are in nm



SiO_2



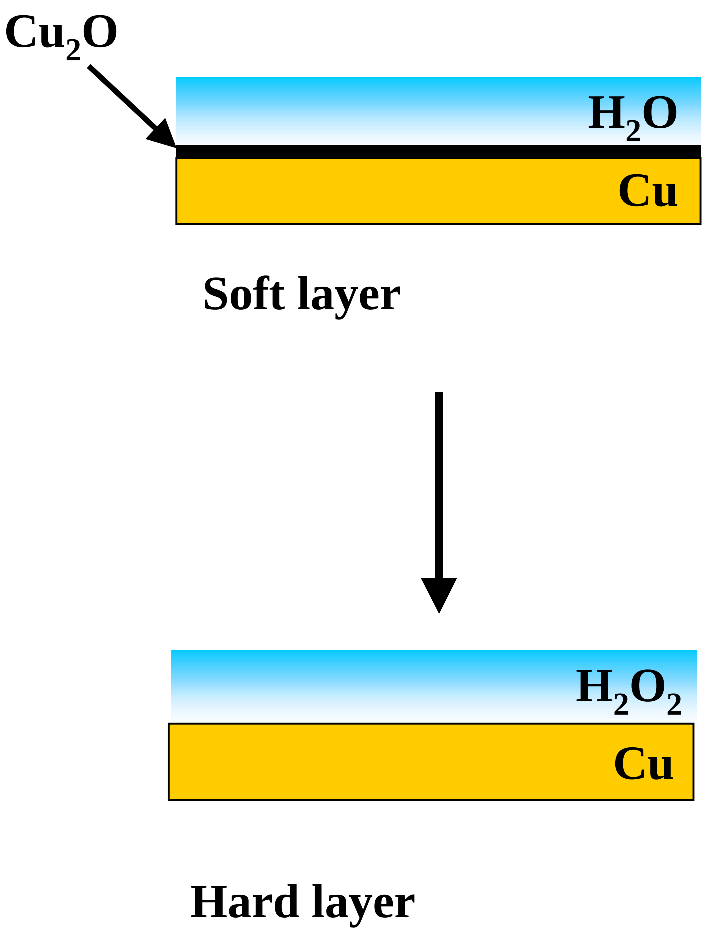
Cu

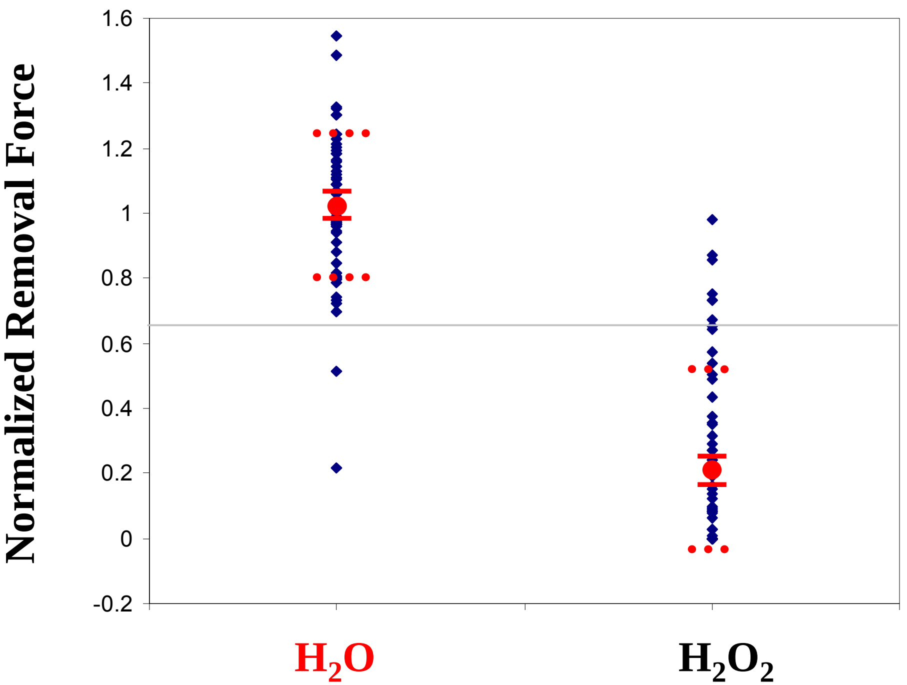


W

Material	ε_s (nm)	Std (nm)	Frac. Coverage	E (Gpa)
SiO_2	1.7	0.7	56	55.8
Cu	0.8	0.5	45	78
W	1.1	.5	41	418
Al_2O_3 particle	1.6	0.7	33	500

CMP and Post-CMP Cleaning – Alumina Particles Interacting with Copper Films

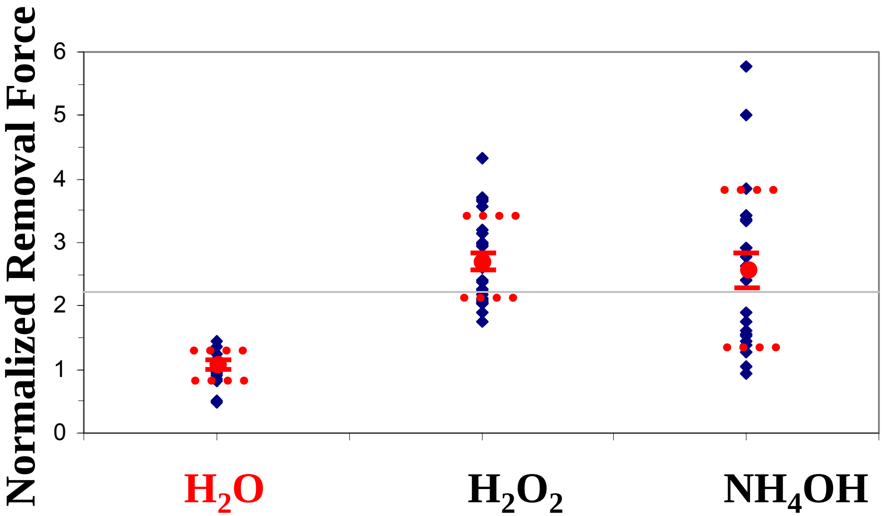




Chemistry	Mean	Std Dev	Std Err Mean
H_2O	1.02	0.22	0.03
H_2O_2	0.25	0.28	0.04

Al_2O_3 particle may also dissolve in acidic solution

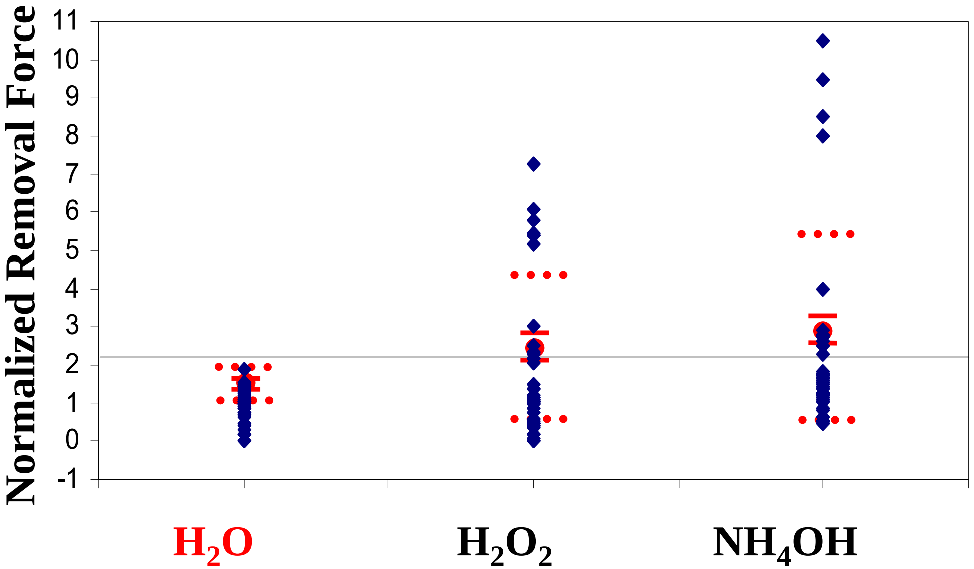
CMP and Post-CMP Cleaning – Alumina Particles Interacting with SiO_2 Films



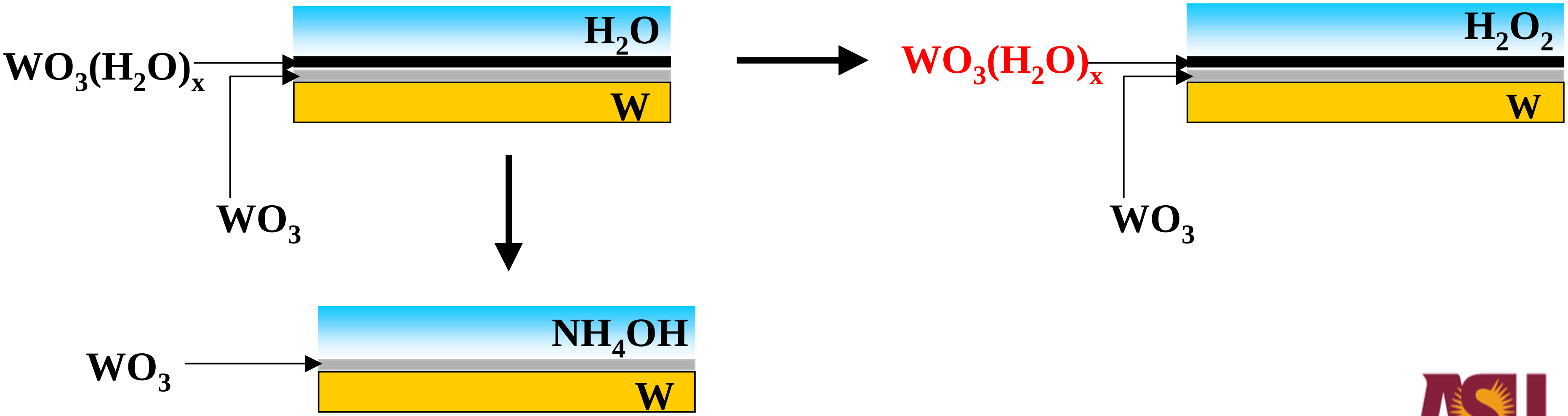
Chemistry	Mean	Std Dev	Std Err Mean
H_2O	1.00	0.23	0.05
H_2O_2	2.72	0.68	0.13
NH_4OH	2.57	1.25	0.26

	SiO_2		Al_2O_3	
	Surface Species	Solubility	Surface Species	Solubility
H_2O	Si-O-Si, =Si(OH), Si(OH)x	$Si(OH)_4$: 10 % dissociation	Al_2O_3	does not dissolve
H_20_2	Si-O-Si, =Si(OH), Si(OH)x	$Si(OH)_4$: 0 % dissociation	Al_2O_3, Al^{+3}	dissolves
NH_4OH	Si-O-Si, =Si(OH), Si(OH)x	$Si(OH)_4$: 100 % dissociation	Al_2O_3, Al^{+3}	dissolves

CMP and Post-CMP Cleaning – Alumina Particles Interacting with Tungsten Films



Chemistry	Mean	Std Dev	Std Err Mean
H_2O	0.96	0.40	0.06
H_2O_2	1.87	1.97	0.29
NH_4OH	2.20	2.26	0.33



Adhesion Model Conclusions

» Expanded existing particle adhesion models to include
  - Chemical and morphological heterogeneities
  - Compression and deformation of surface asperities
  - Non-ideal geometries

» Obtained statistical information on particle adhesion

» Developed experimental procedure to measure particle adhesion for different particle/substrate systems as a function of
  - Aqueous environment
  - Contact time
  - Applied load
  - Solution temperature

Removal Model Objective

Assess mechanism(s) of micron-scale particle removal from semiconductor wafer surfaces using a critical particle Reynolds number approach

- Relate adhesion models to particle removal
- Relate flow characteristics to particle removal
- Develop model for removal processes by combining adhesion and flow models
    - Determine effect of Hamaker constant (A) on model
    - Determine effect of particle size distribution on model
    - Determine effect of roughness on model

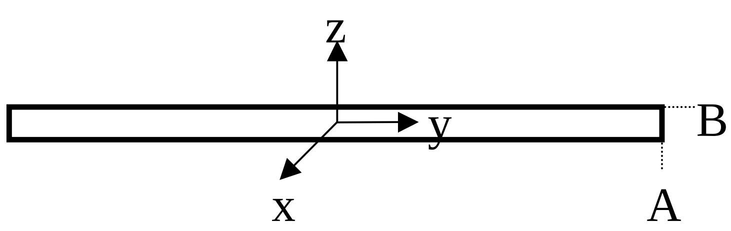
Preliminary Work

Use experimental results from Yiantsios and Karabelas *J. of Colloid and Interface Sci.* 176, 74-85 (1995) to assess validity of critical particle Reynolds number approach

- Studied detachment of spherical glass particles from a flat glass surface
- Used laminar channel flow over a range of flow rates to remove adhering particles
- Percentage adhering as a function of wall shear stress (τ_w) presented graphically
- System Properties
  - › Fluid: solution of distilled water, HNO_3, and $NaNO_3$
    - Ionic strength: 1×10^{-3} mol/L
    - pH: 3
  - › Particle (mean) diameters: 2, 5, 10, 15 μm (σ ~ 12%)
  - › Estimated maximum roughness of surface: 0.8 nm
  - › Hamaker constant (A): 1.14×10^{-20} J

Flow System †

Front View



Flow Properties

- Flow Rates: 0.02 – 25 cm^3/s
- Re: 4 – ~5000
- Type of Flow: laminar
- Velocity in x-direction only: u = u(y,z)
- Boundary Conditions:

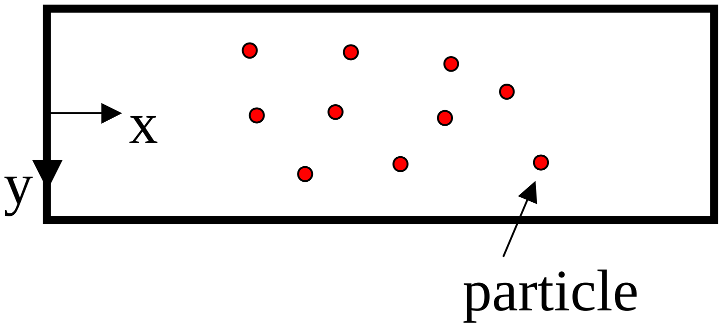
$$u(B,-A) = u(B,A) = 0$$

$$u(-B,-A) = u(-B,A) = 0$$

Channel Dimensions

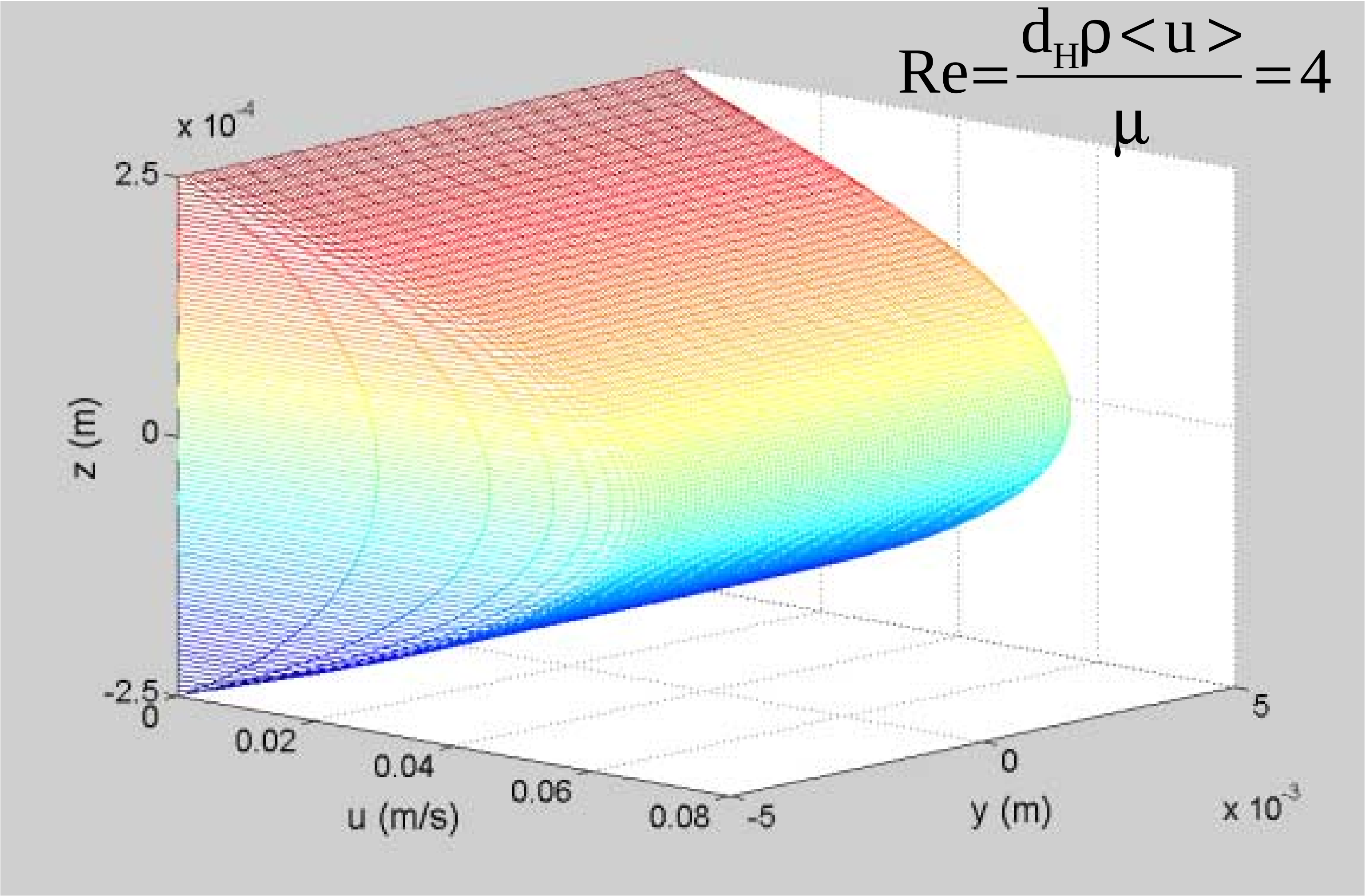
- Width (2A): 1 cm
- Height (2B): 0.5 mm
- Hydraulic Diameter (d_H): 0.952 mm

Top View

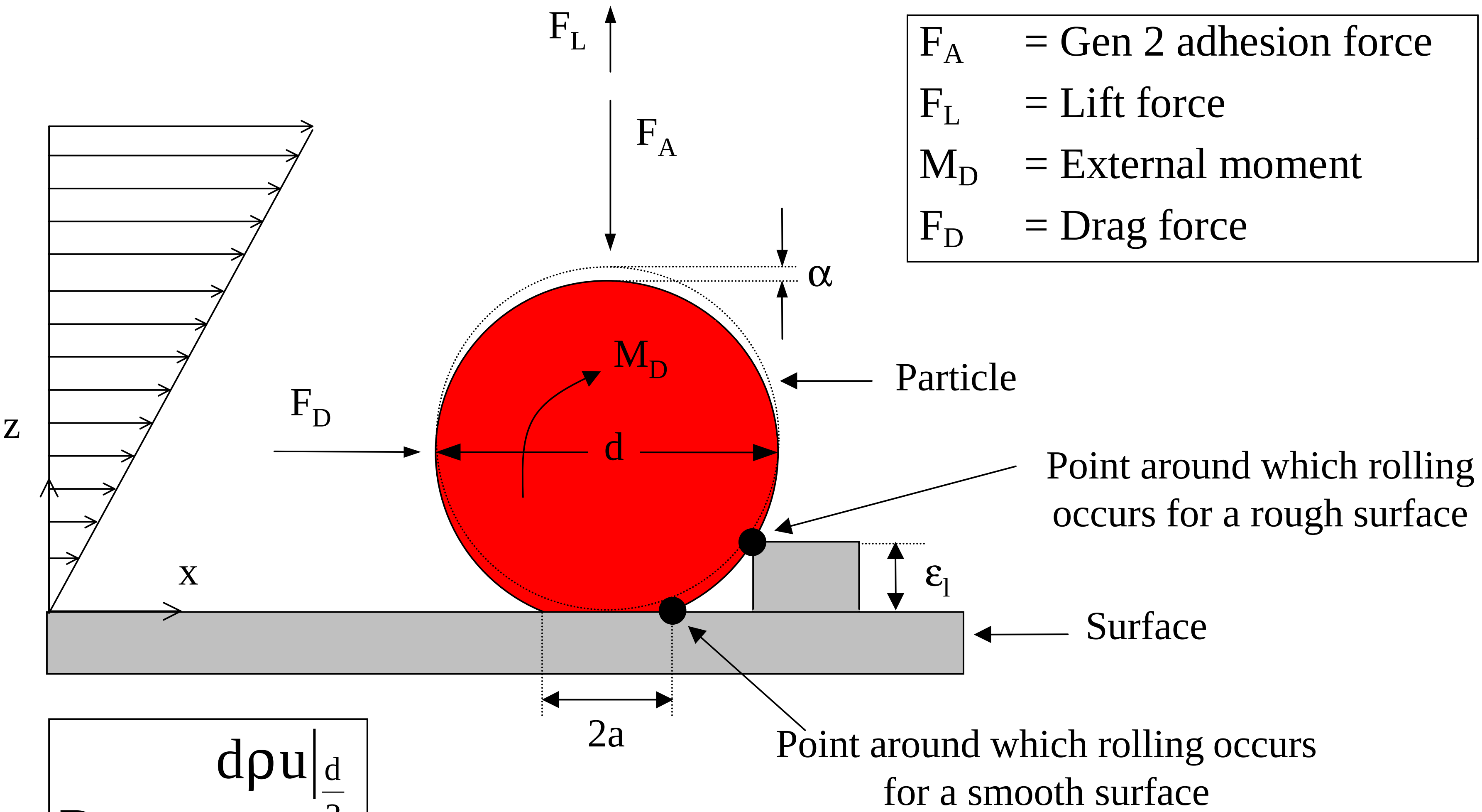


† *J. Colloid Interface Sci. 176, 74-85 (1995)*

Velocity Profile, Q = 0.02 cm^3/s



Particle Adhesion/Removal Model



F_A = Gen 2 adhesion force
F_L = Lift force
M_D = External moment
F_D = Drag force

$$Re_p = \frac{d\rho u\big|_{\frac{d}{2}}}{\mu}$$

Rolling Particle Removal Criteria

$$\overline{M}_D + \overline{F}_D \cdot l_1 + \overline{F}_L \cdot l_2 \geq \overline{F}_A \cdot l_2$$

Vertical lever arm

Lift force

$$F_L \propto d \left.\frac{du}{dz}\right|_{\frac{d}{2}} Re_p$$

Horizontal lever arm

Drag force

$$F_D(Re_p < 1) \propto Re_p$$

Adhesion force

$$F_A \propto Ad$$

External moment of surface stresses about center of particle

$$M_D \propto d\, Re_p$$

Assessing Particle Removal

- » Removal occurs when Re_p(Flow) ≥ Re_{pc}(Rolling)

  Re_p(Flow) constant at constant flow rate (for this system)

- » ***Ideal system*** of smooth, deformable spherical particles of identical radius adhering to a smooth, flat, deformable surface

  → Single adhesion force

  ⇒ Single value of Re_{pc}

  ⇒ All or none of the adhering particles should be removed

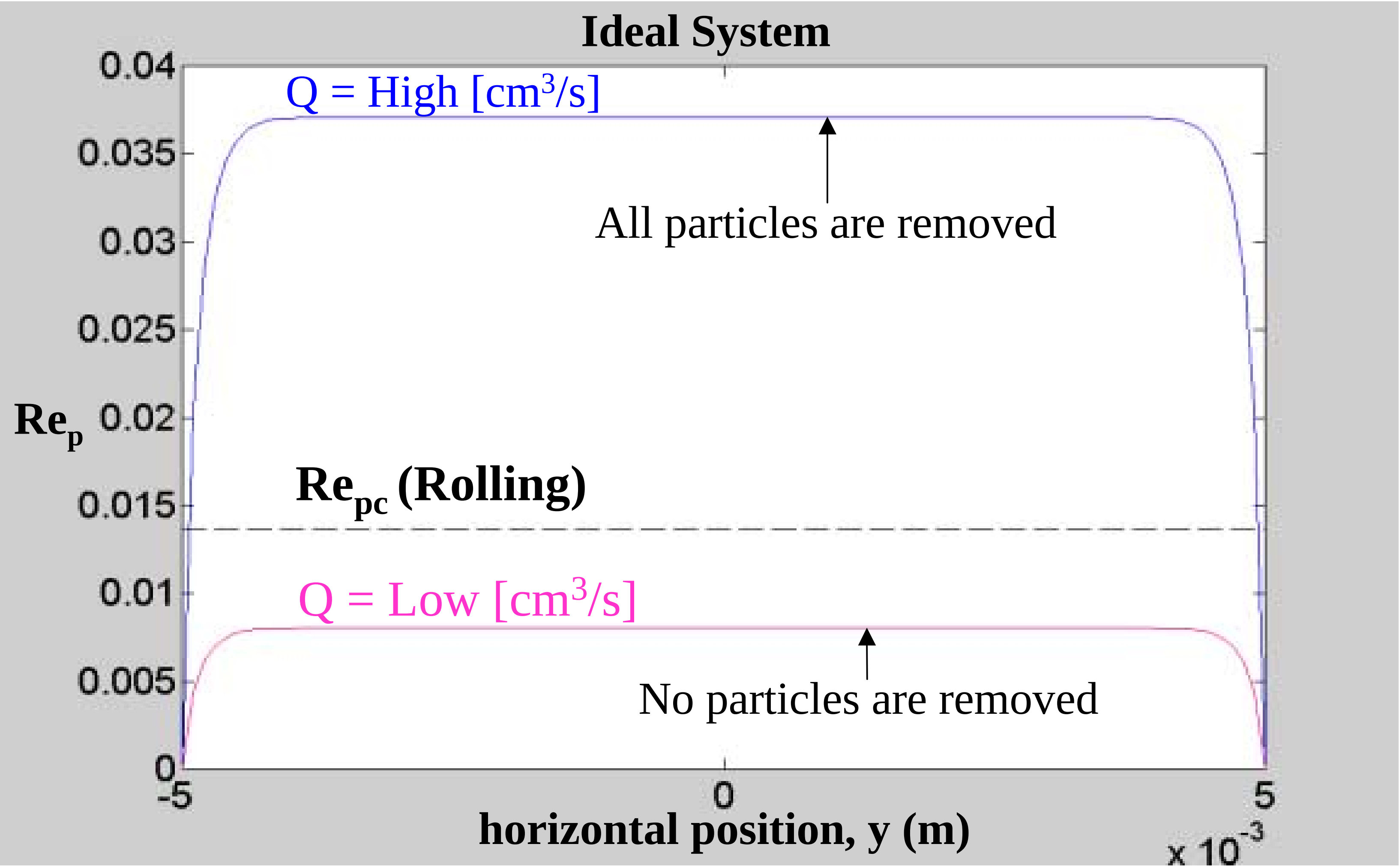
- » ***Real system*** of deformable particles with non-uniformly distributed roughness and a finite size distribution adhering to a deformable surface with a non-uniform roughness distribution

  → Multiple adhesion forces and multiple points around which rolling can occur

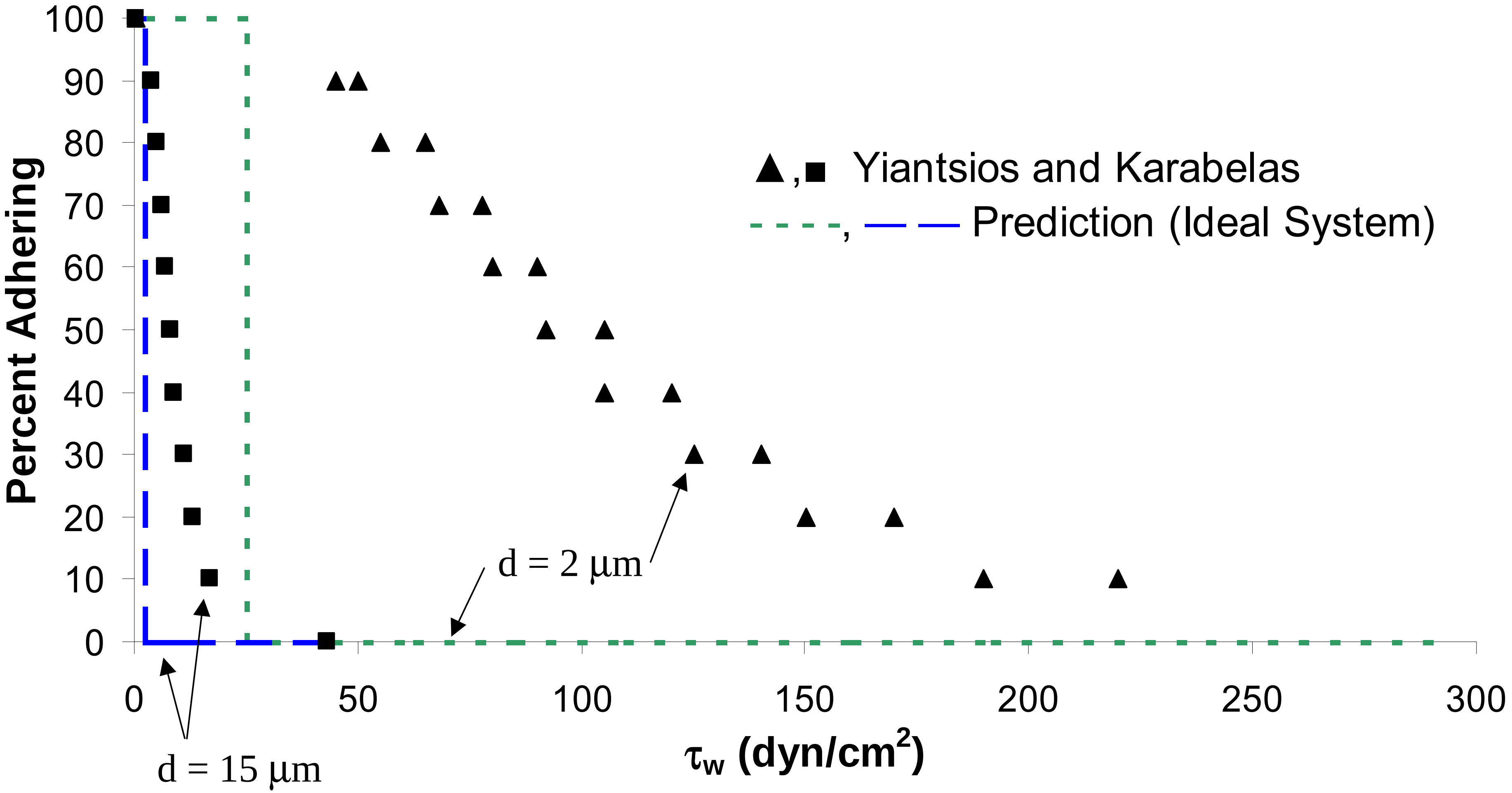
  ⇒ Multiple values of Re_{pc}

  ⇒ All, some, or none of the adhering particles can be removed

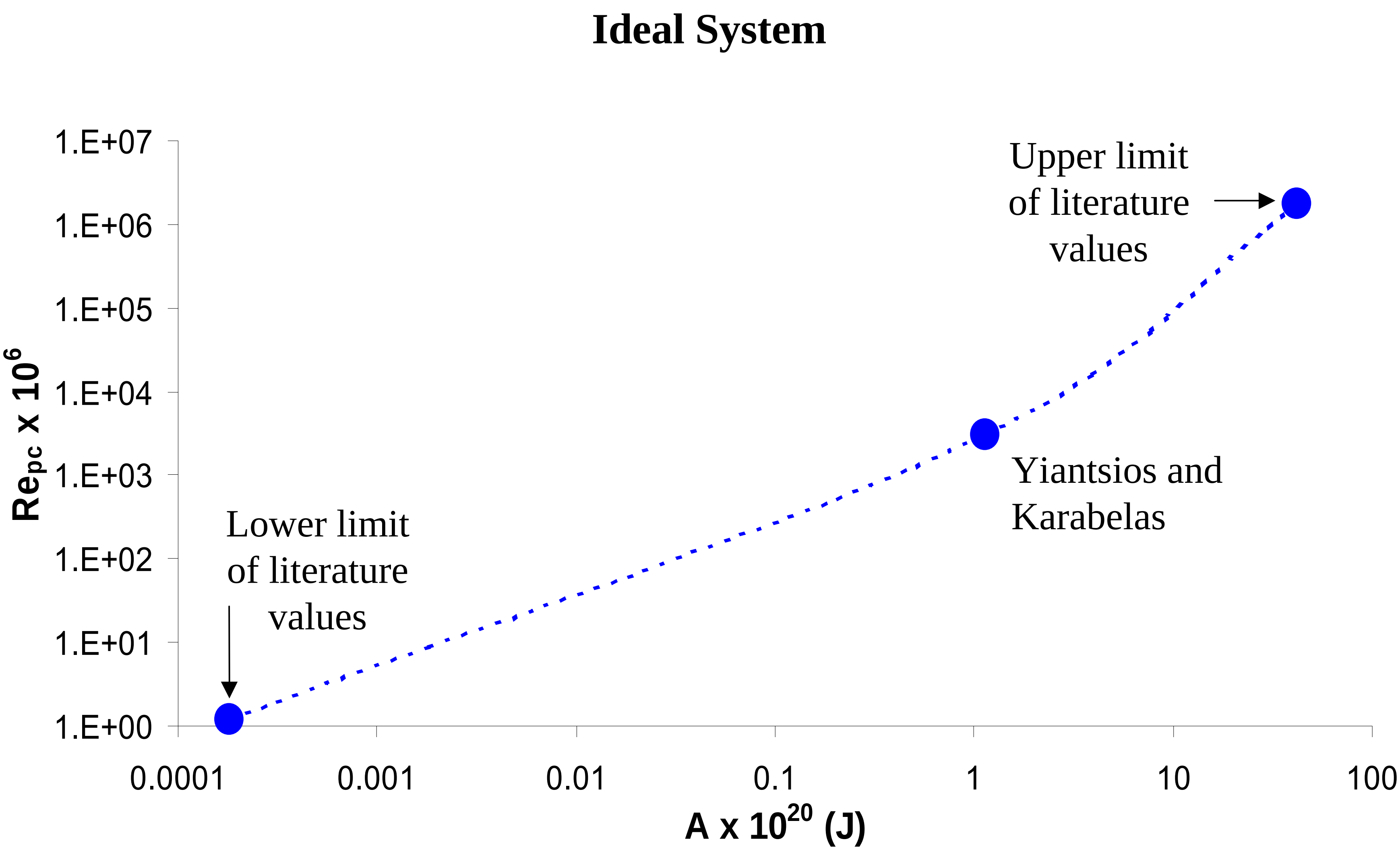
Illustration: Critical Particle Reynolds Number Approach



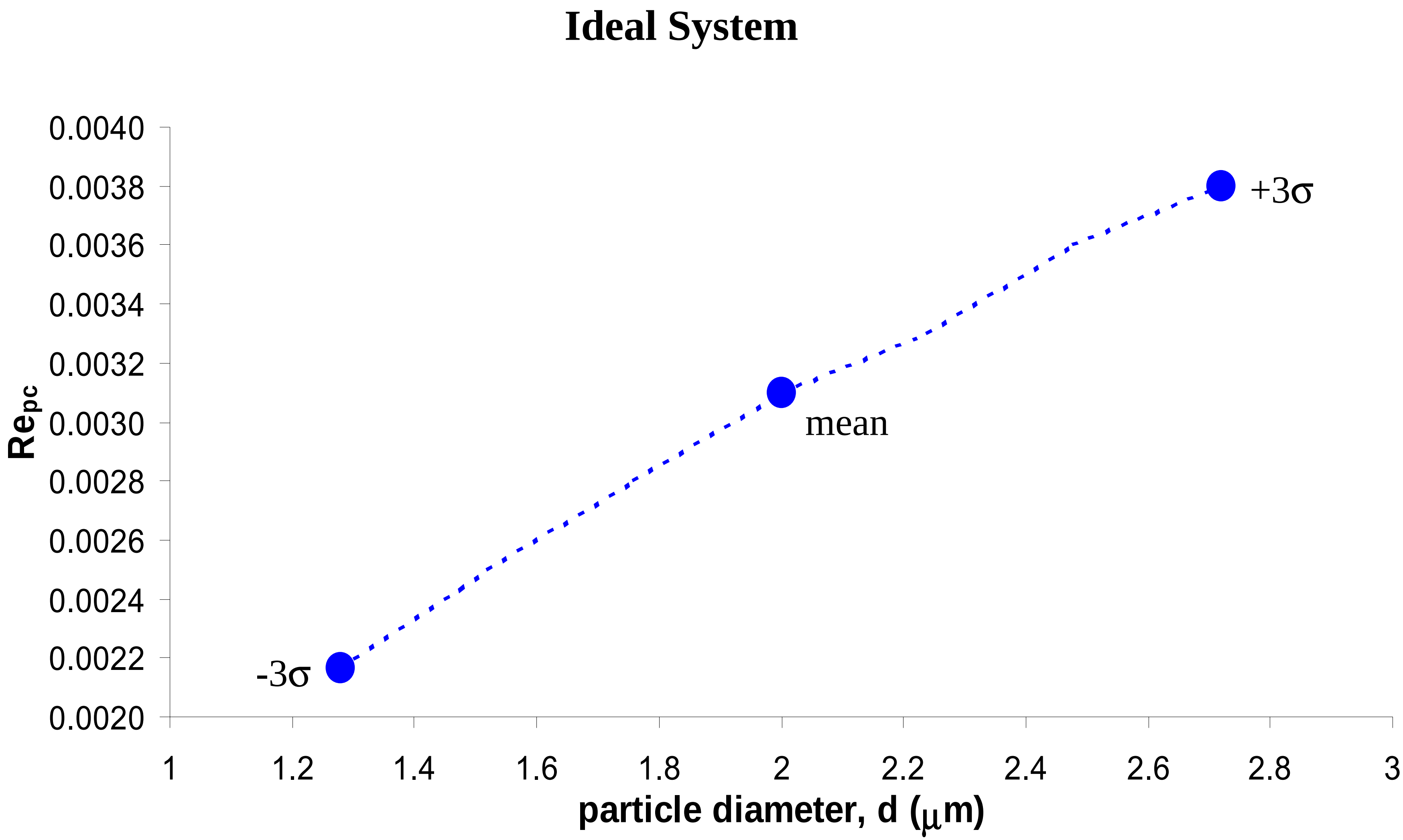
Adhesion Profile, d = 2 and 15 μm



Effect of Hamaker Constant on Re_{pc}, d = 2 μm



Effect of Particle Size Distribution on Re_{pc}



Effect of Roughness on Adhesion Force

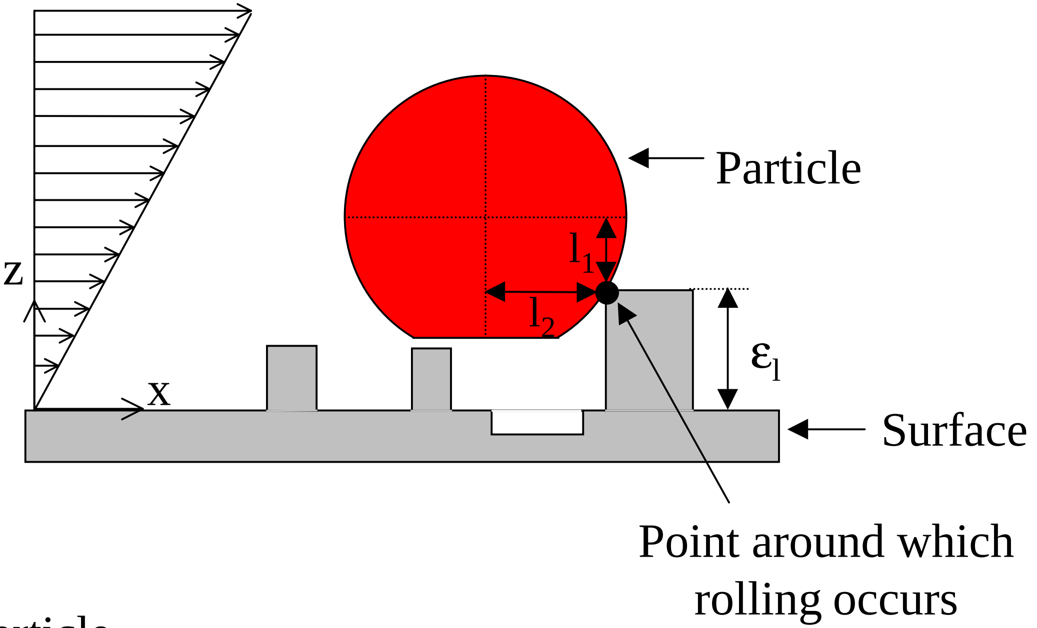
System **d = 2 μm A = 1.14 x 10^{-20}J**	**Mean F_A (N)**	**Standard Deviation**
Ideal Smooth particle/Smooth surface	1.3 x 10^{-8}	-
Real Rough particle/Rough surface	2.2 x 10^{-9}	3.1 x 10^{-11}

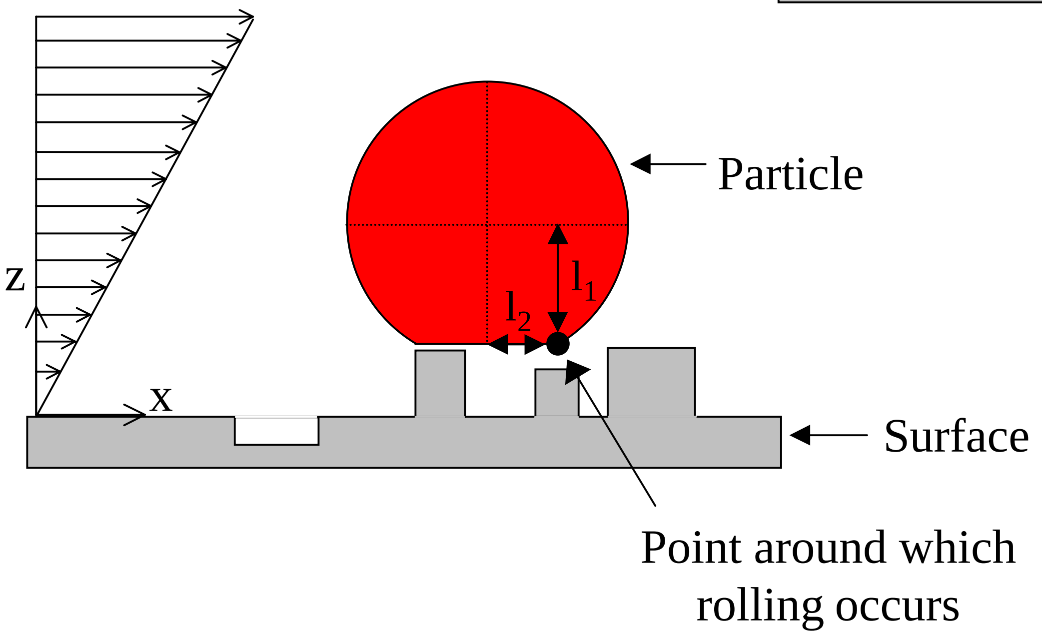
Assumptions for Roughness			
	Average Height (nm)	**Standard Deviation (nm)**	**Fractional Coverage**
Particle	0.4	0.4	0.25
Surface	0.4	0.4	0.25

Effect of Roughness on Re_{pc}

Roughness affects Re_{pc} by affecting

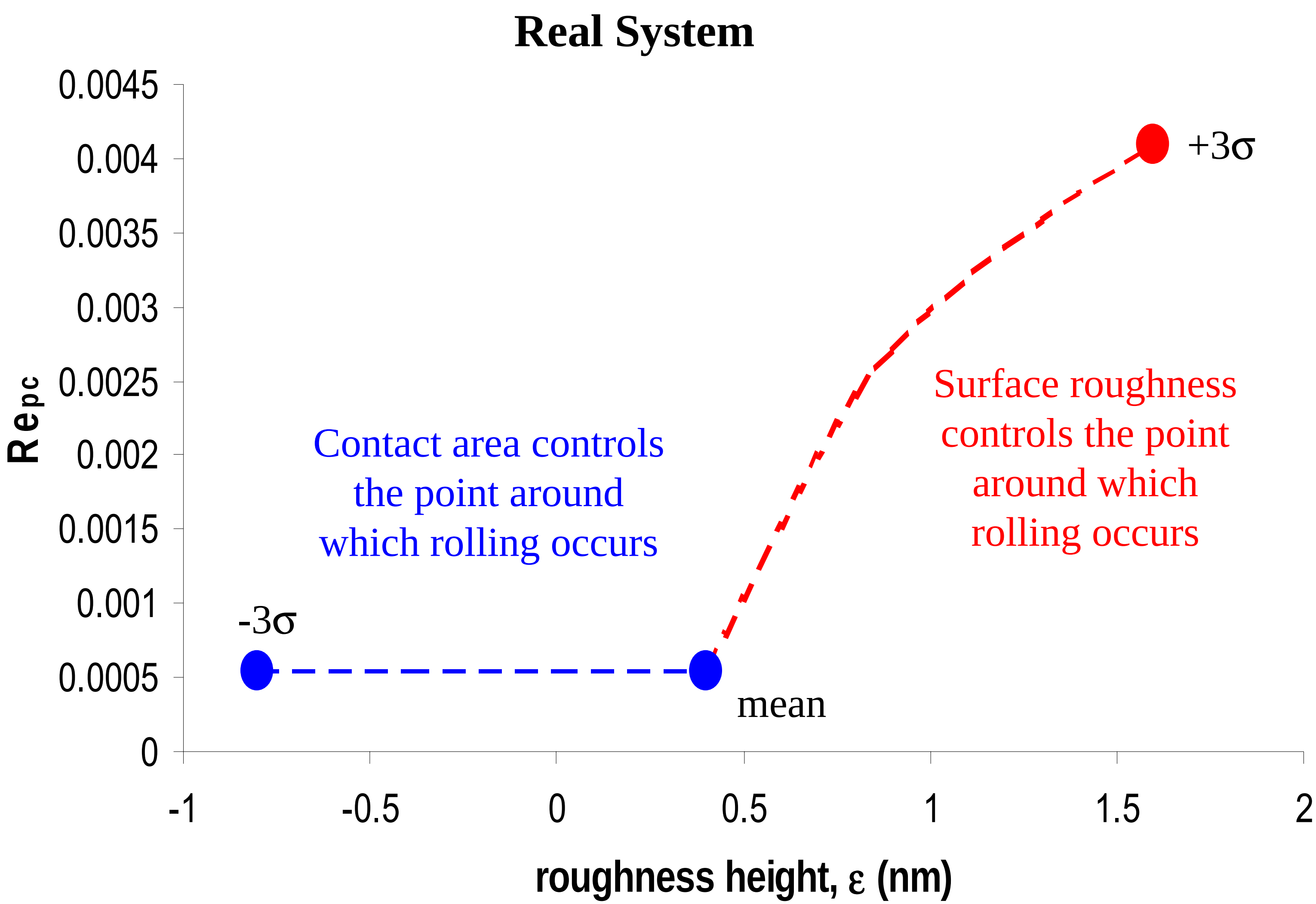
- Adhesion force
- Point around which rolling can occur



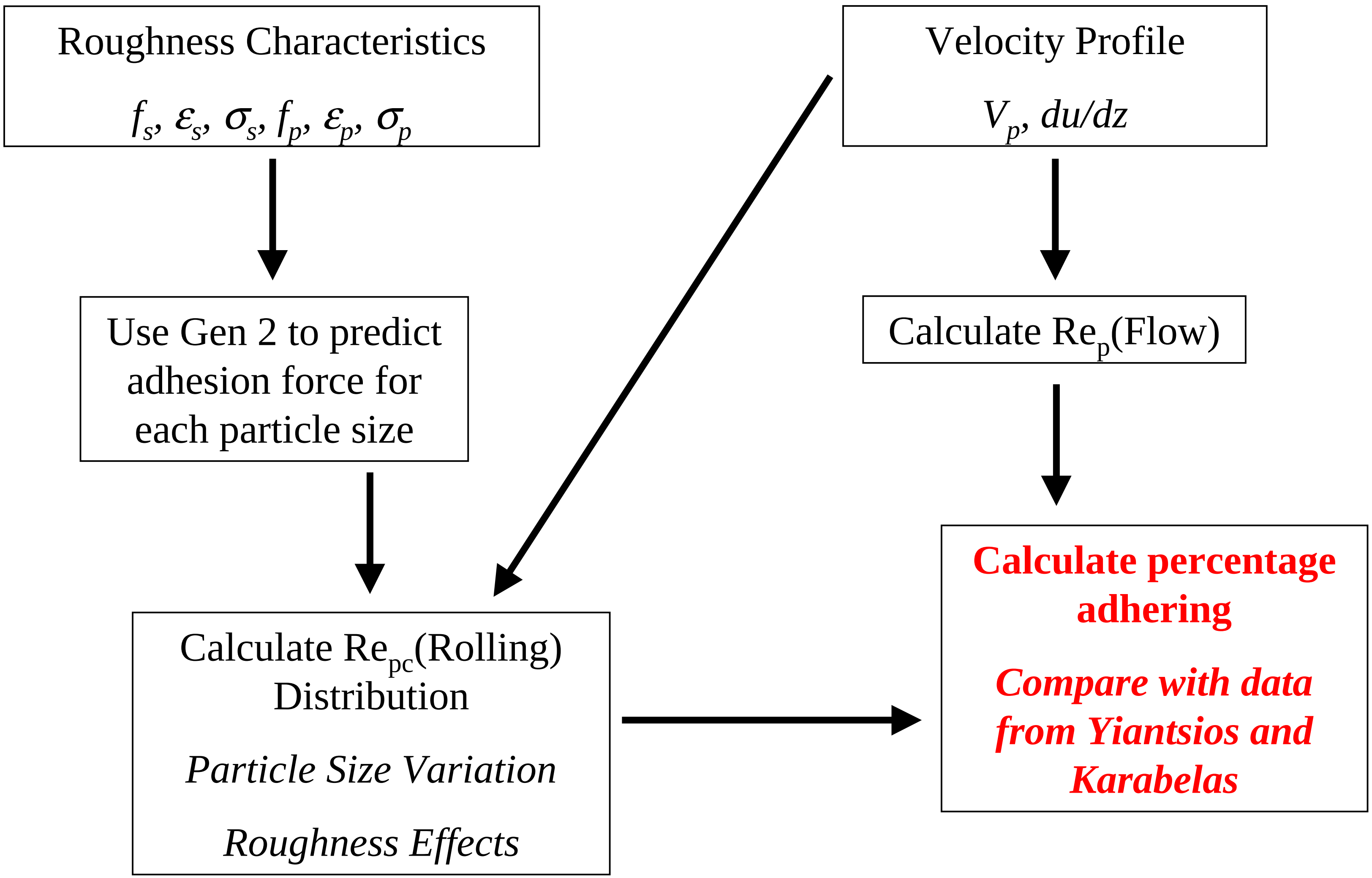


Length of horizontal and vertical lever arms (l_1 and l_2) depend on ε_l

Effect of Roughness on Re_{pc}, d = 2 μm



Removal Analysis Procedure



Calculating the Adhesion Force using Gen 2, d = 2 μm

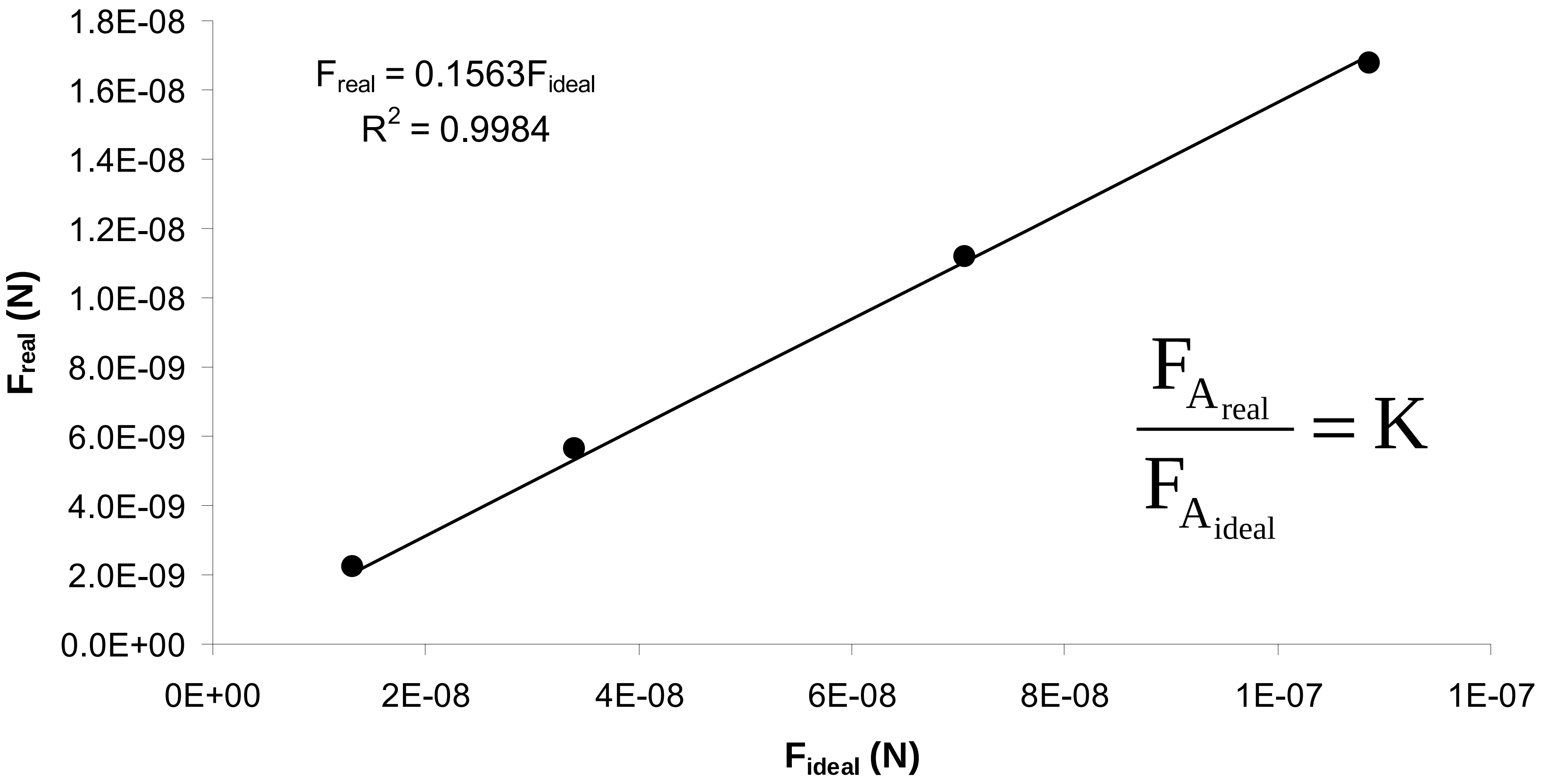
Parameter	Value
Hamaker constant (A)[1]	1.14×10^{-20} J
Lennard-Jones separation distance (D_{LJ})[2]	0.4 nm
Bulk modulus (E)[1]	4.86×10^{10} N/m^2
Applied load (P) = weight of particle[2]	1.03×10^{-13} N
Fraction of surface covered with asperities (f_s)[3]	0.25
Average roughness height on surface (ε_s)[3]	0.4 nm
Standard deviation in surface roughness height (σ_s)[3]	0.4 nm
Fraction of particle covered with asperities (f_p)[3]	0.25
Average roughness height on surface (ε_p)[3]	0.4 nm
Standard deviation in surface roughness height (σ_p)[3]	0.4 nm
Contact radius (a), calculated using the DMT theory	6.46 nm

[1]Taken from Yiantsios and Karabelas

[2]Set by Gen 2

[3]Estimated values based on information given by Yiantsios and Karabelas

Calculating the Adhesion Force using Gen 2



$$\frac{F_{A_{real}}}{F_{A_{ideal}}} = K$$

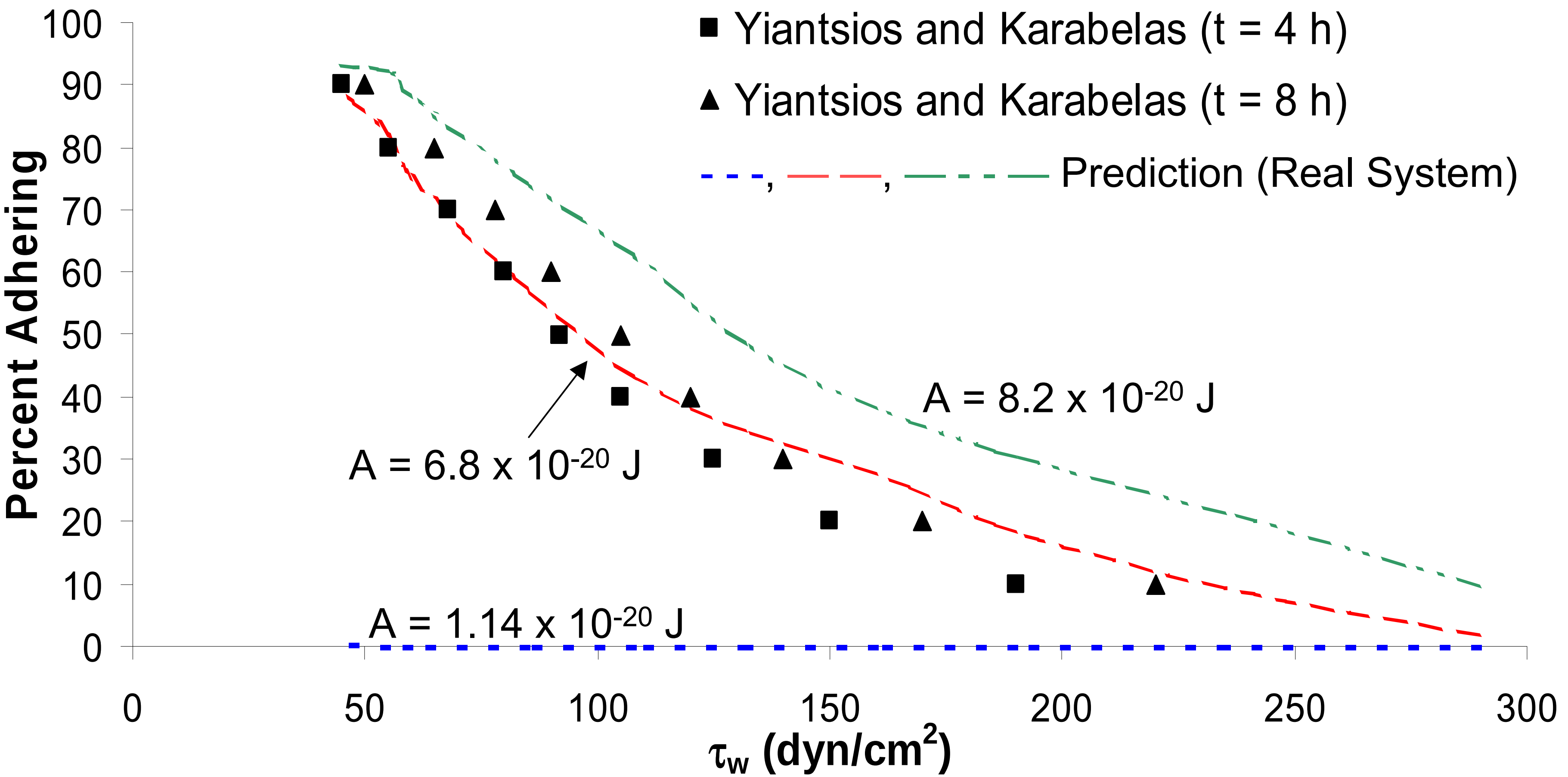
Calculating the Adhesion Force using Gen 2

$$F_{A_{real}}(A, D, E, P, f_s, \varepsilon_s, \sigma_s, f_p, \varepsilon_p, \sigma_p, a) \qquad \frac{F_{A_{real}}}{F_{A_{ideal}}} = K$$

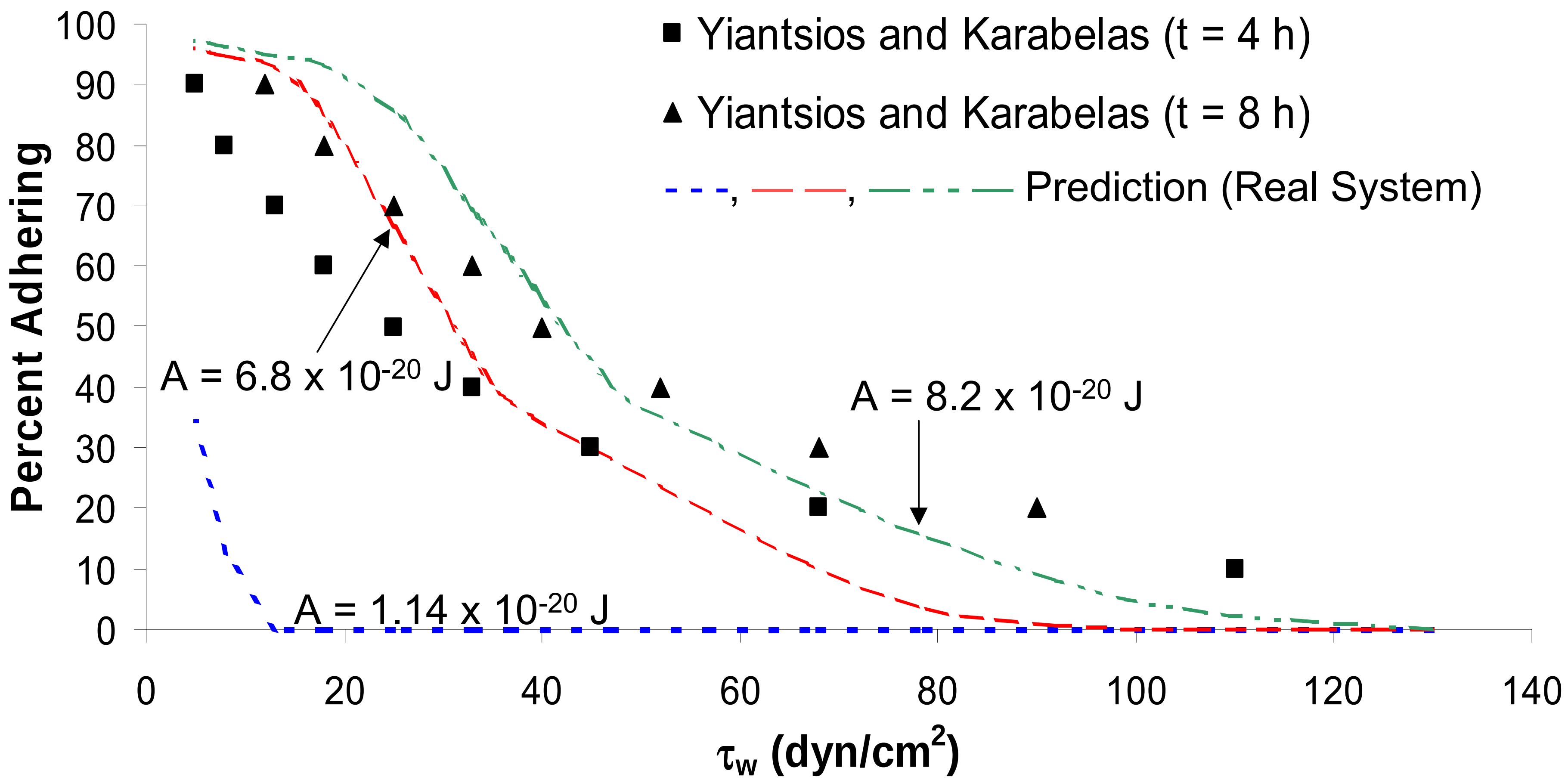
$$F_{A_{real}}(A, \varepsilon_s, \varepsilon_p) = K(\varepsilon_s, \varepsilon_p) \cdot F_{A_{ideal}}(A)$$

A, ε_s, ε_p have the most influence on the adhesion force for this system

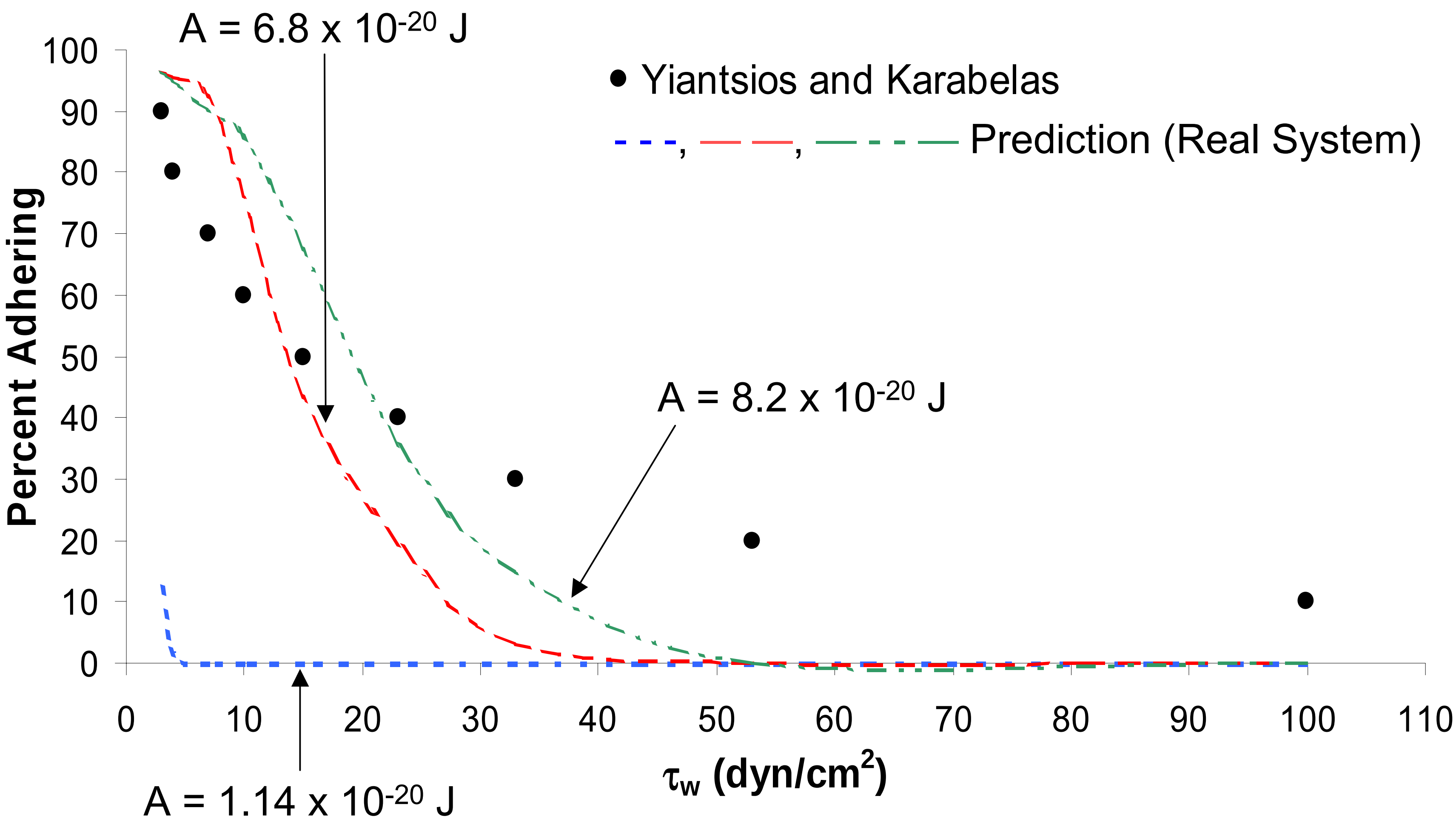
Adhesion Profile, d_{mean} = 2 μm



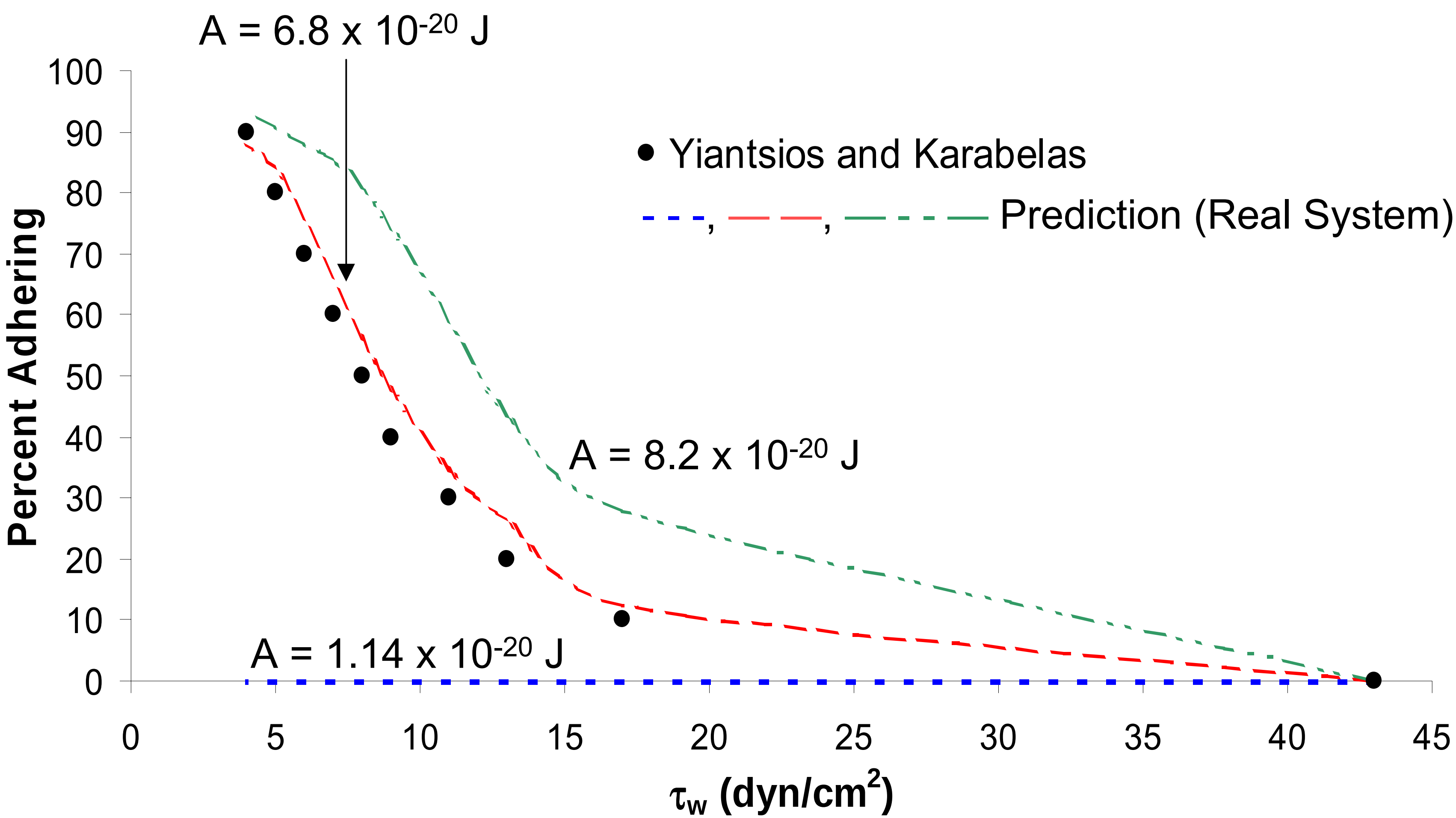
Adhesion Profile, d_{mean} = 5 μm



Adhesion Profile, d_{mean} = 10 μm



Adhesion Profile, d_{mean} = 15 μm



Removal Model Conclusions

- » Accurate particle removal models require accurate particle adhesion models
  - Removal is highly dependent on adhesion model through
    - › Particle size distribution
    - › Roughness
    - › Hamaker constant
- » Rolling is the controlling removal mechanism
- » Roughness and particle size distribution affect the point around which rolling can occur
- » (Rolling) theoretical adhesion profiles for real adhesion system in agreement with those of Yiantsios and Karabelas
- » Critical particle Reynolds number approach validated
- » Predictive model for particle removal established

  Independent of particle size and cleaning (flow) system

Ongoing Work

Use channel flow system to experimentally validate removal model (critical Reynolds number approach)

- Vary particle diameter, particle composition, fluid flow rate, and fluid viscosity
- Experimentally measure adhesion force and Hamaker constant
- Experimentally determine particle and surface roughness
- Determine effect of roughness on particle adhesion (through validated models)

Future Work

- » Use critical particle Reynolds number approach for
  - Asymmetrical particle analysis
  - Embedded particle analysis
  - Effect of particle agglomeration on removal
  - Tool based studies
    - › Brush scrubbing
    - › Megasonic cleaning
- » Determine effect of turbulent flow on particle removal
- » Use results in fab to optimize post-CMP cleaning

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