Describing Roughness During Contact Sampling:

Statistical Considerations for Swab Screening Explosive Particulates

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Trace Explosives Sensing for Security Applications – II (TESSA02)
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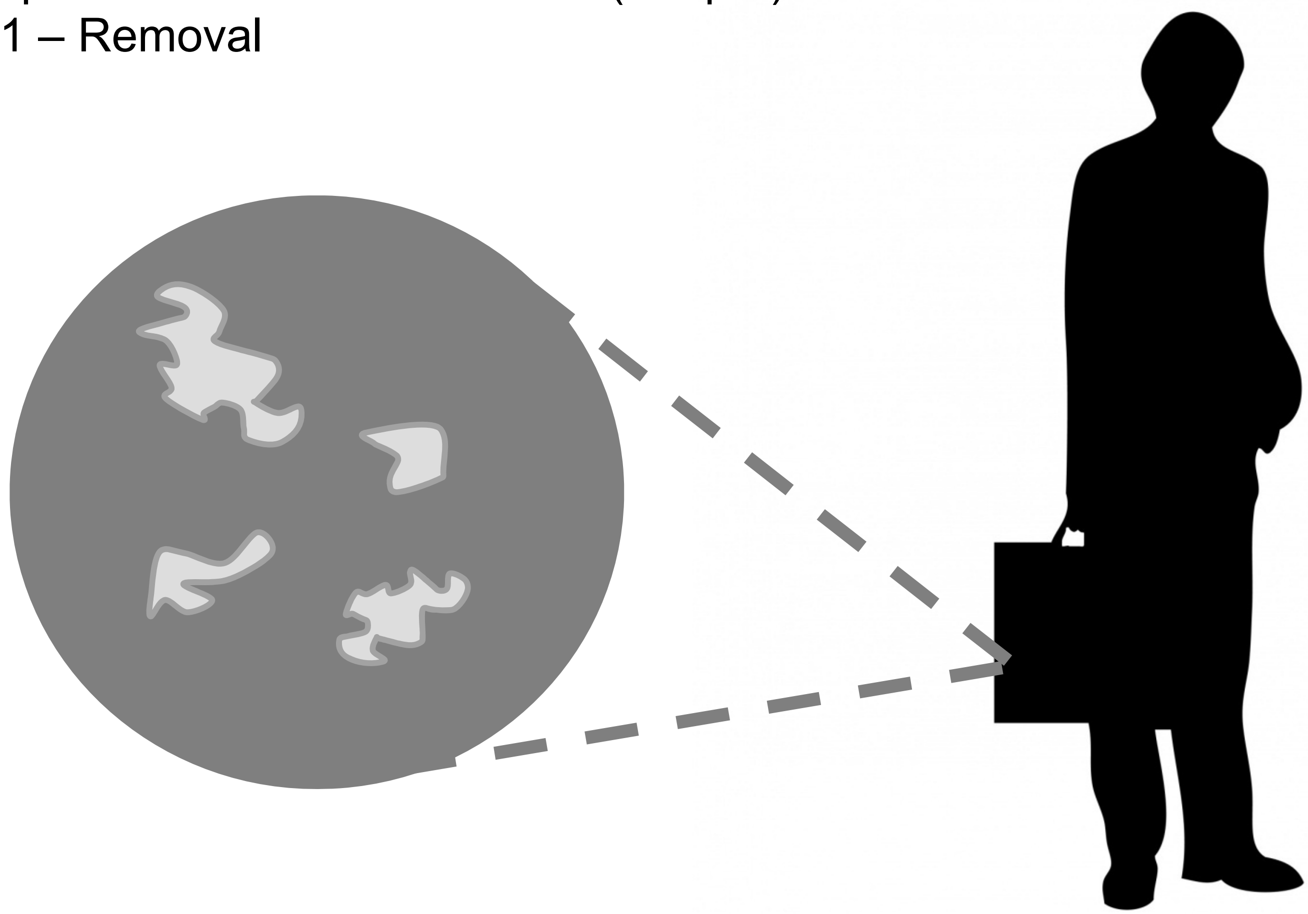
Swab Sampling

Trace Explosive Sampling

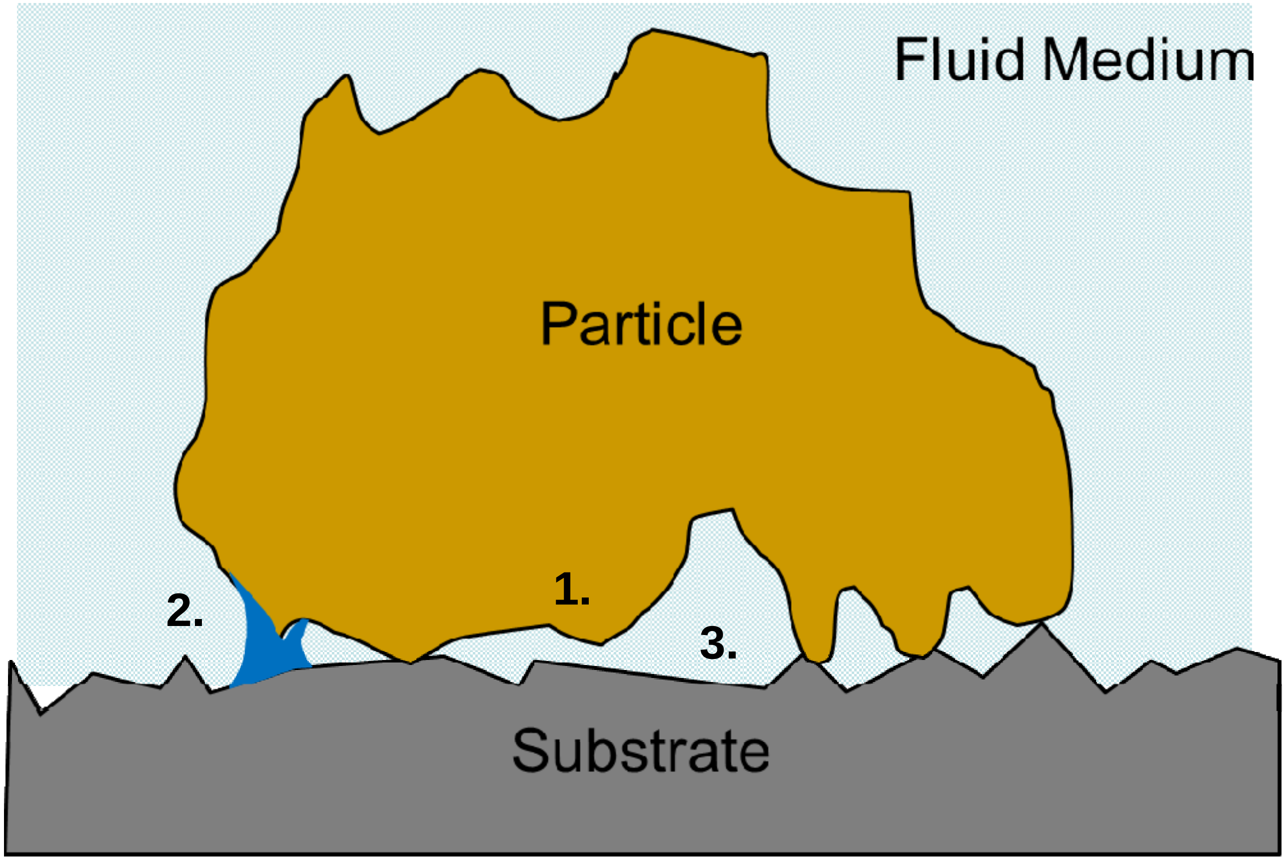
- Ion Mobility Spectrometer (IMS)
- Trace particulates ~order of 10^{-5}m (~50µm)
- Step 1 – Removal



Adhesion

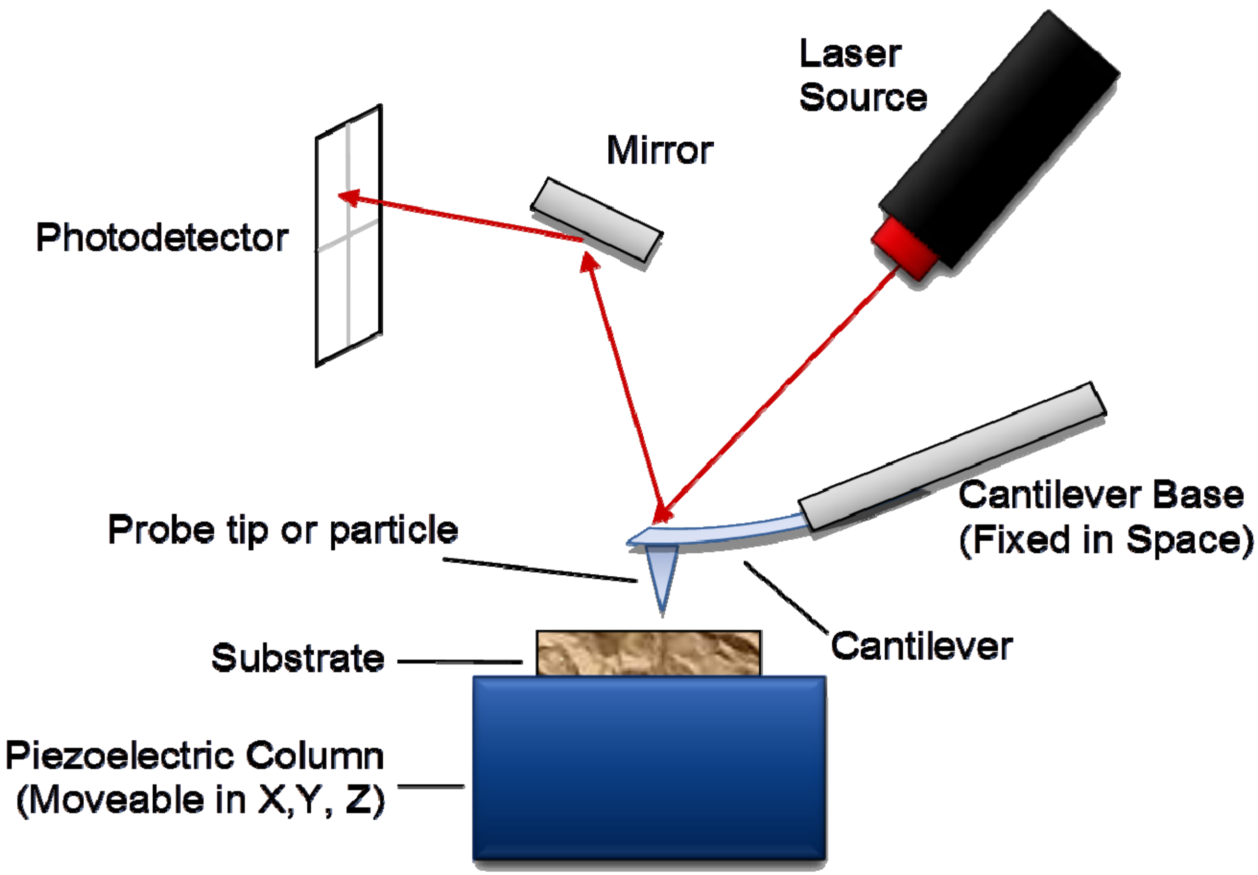
Three Primary Intermolecular Forces

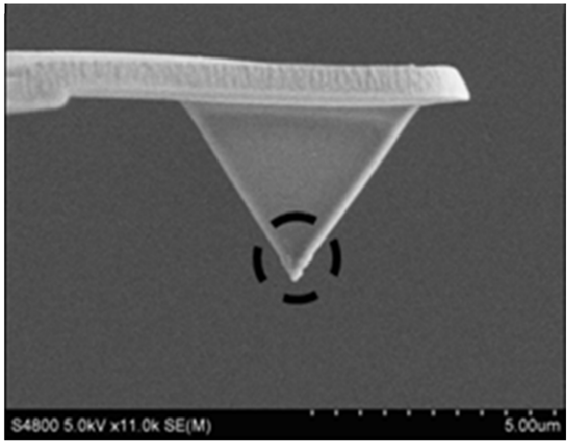
1. van der Waals (vdW)
2. Capillary
3. Electrostatic

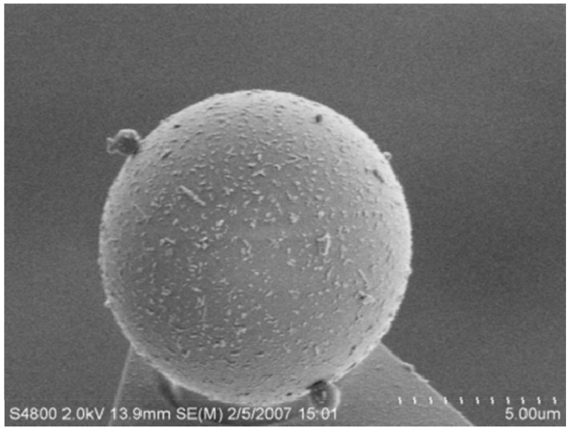


Measuring Adhesion

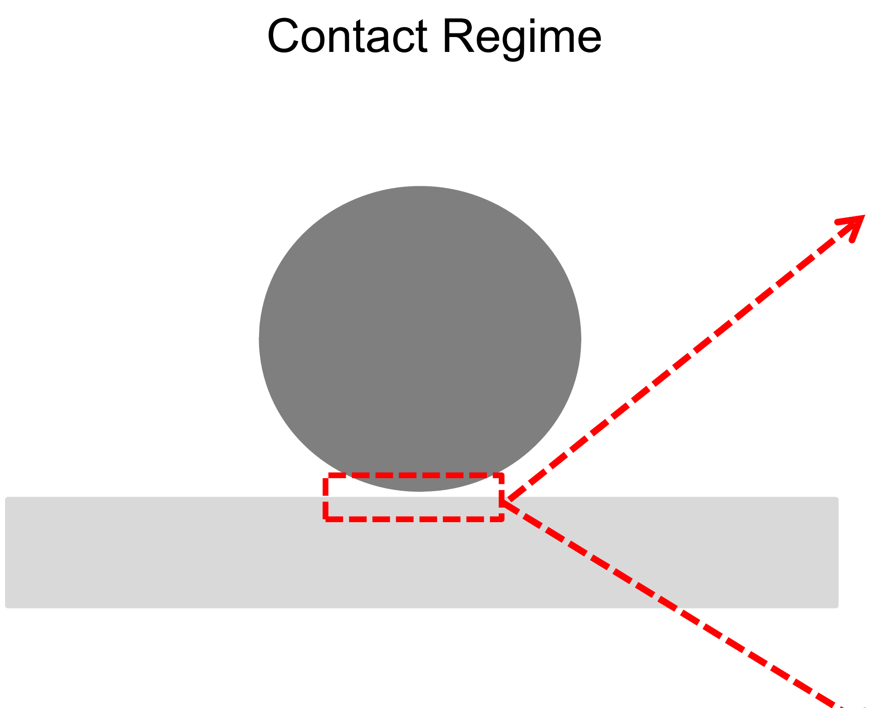
Atomic Force Microscopy

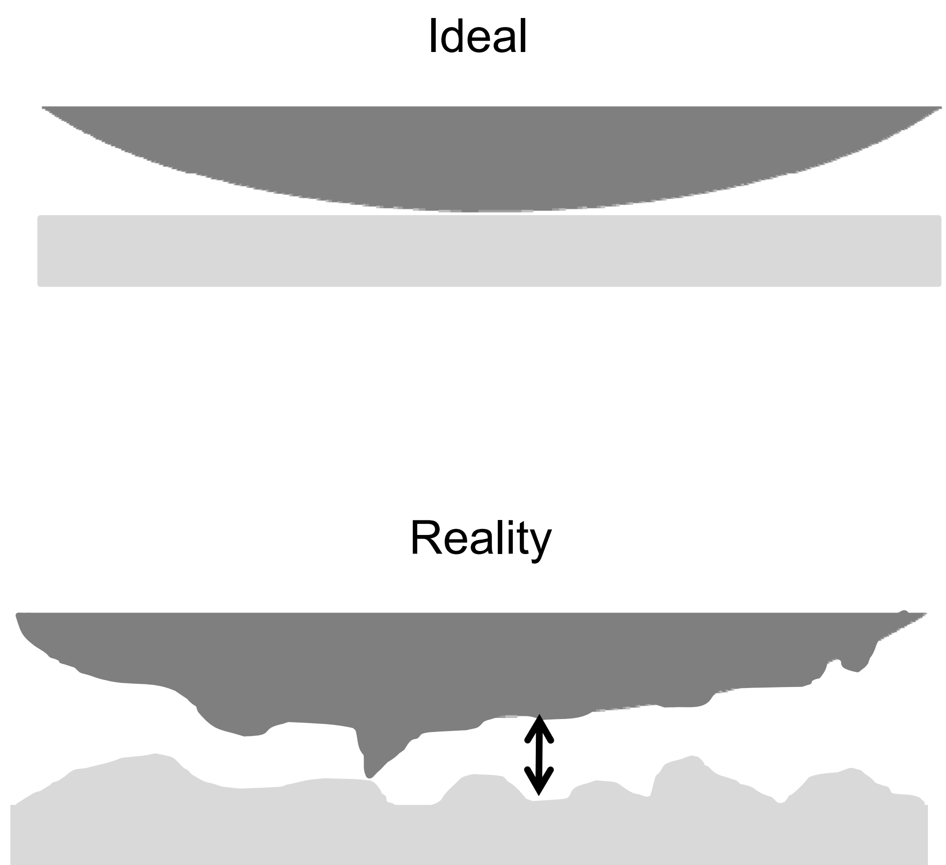






Modeling Adhesion – Surface Roughness



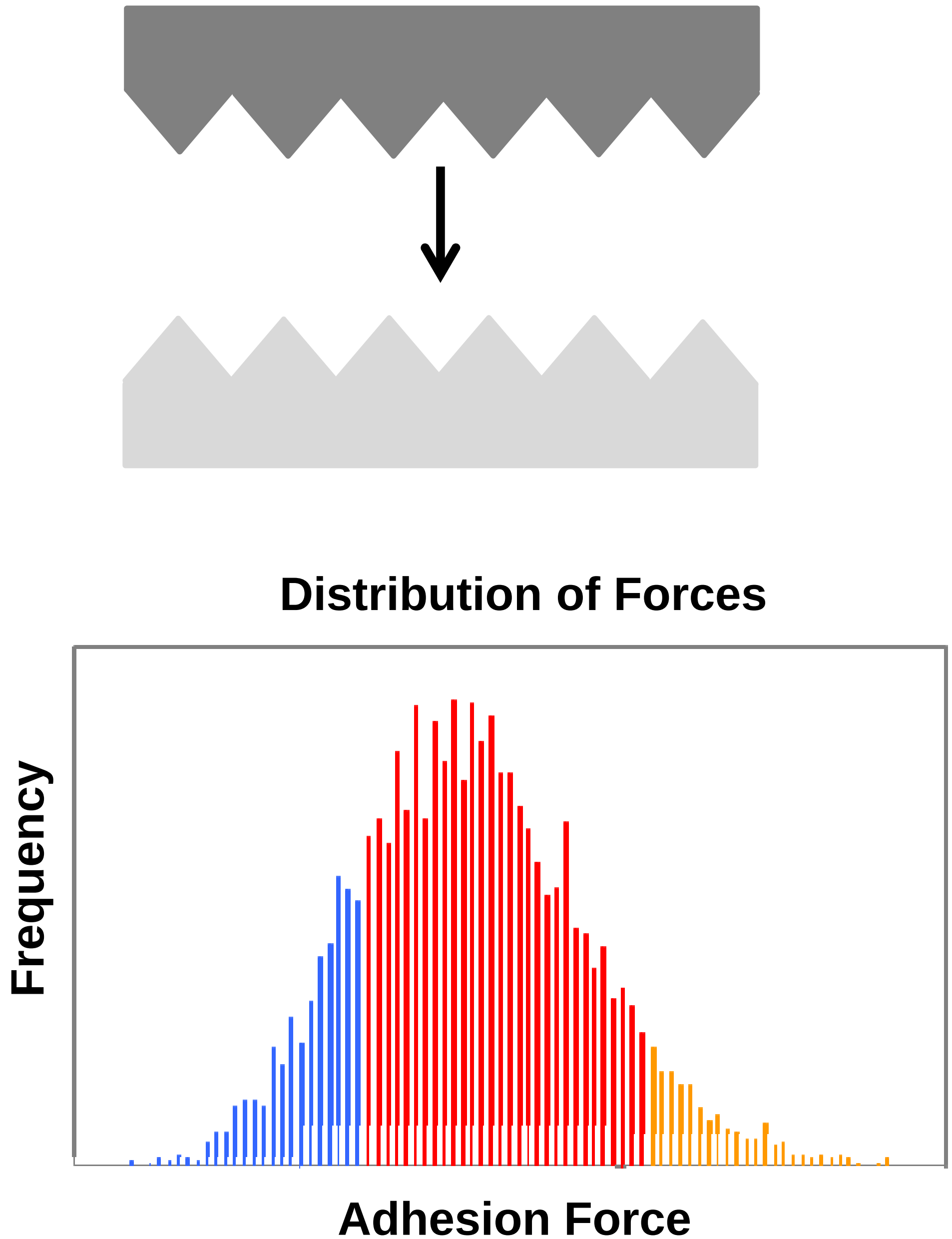


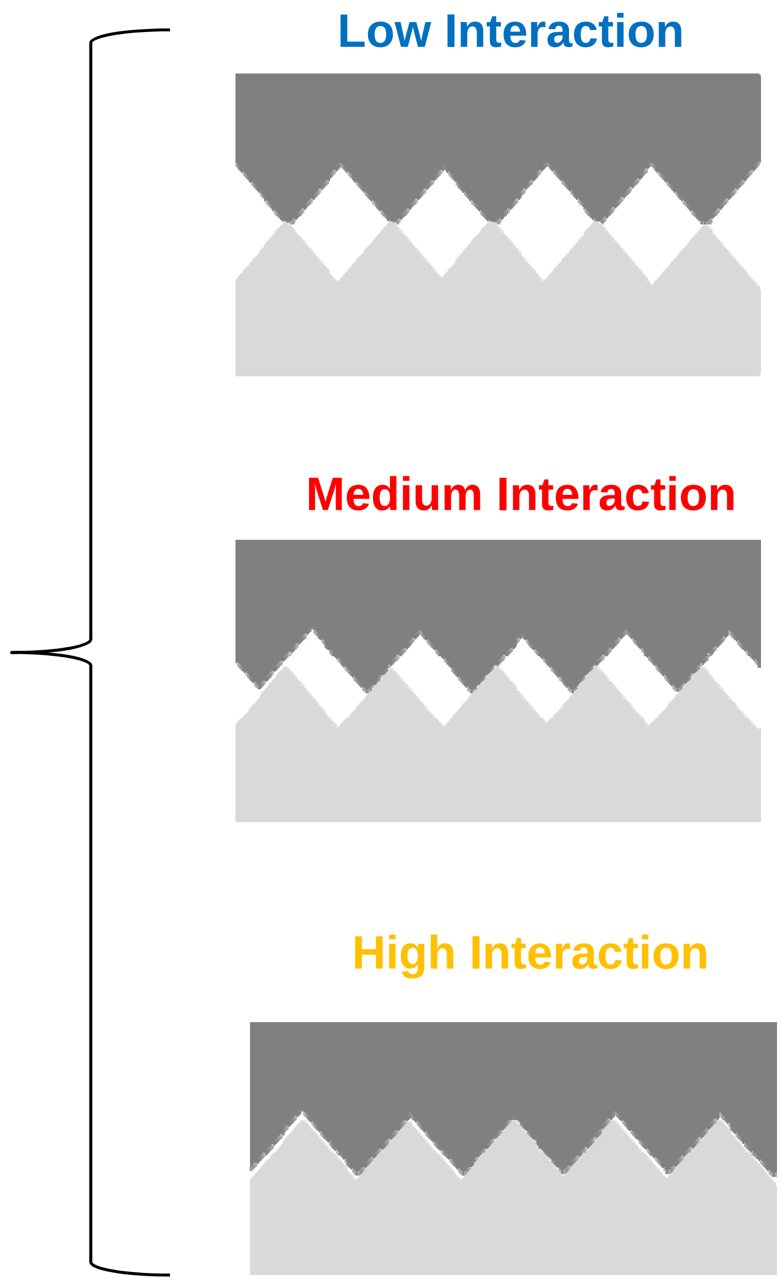
$$F_{sphere-plate}(z) = -\frac{AR}{6z^2}$$

Surface Roughness

1. Decreases material in vdW contact
2. Increases variability of contact measurements

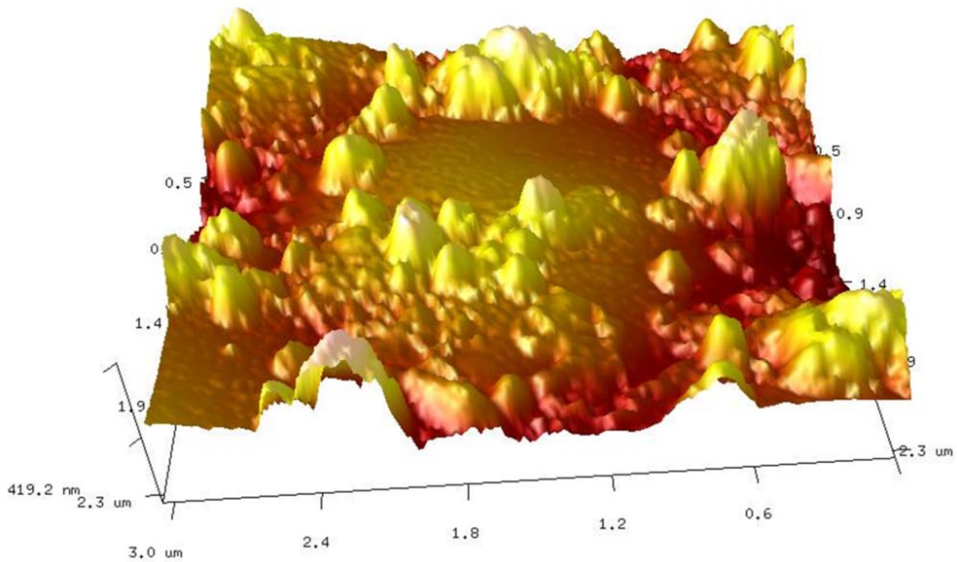
Distribution of Forces



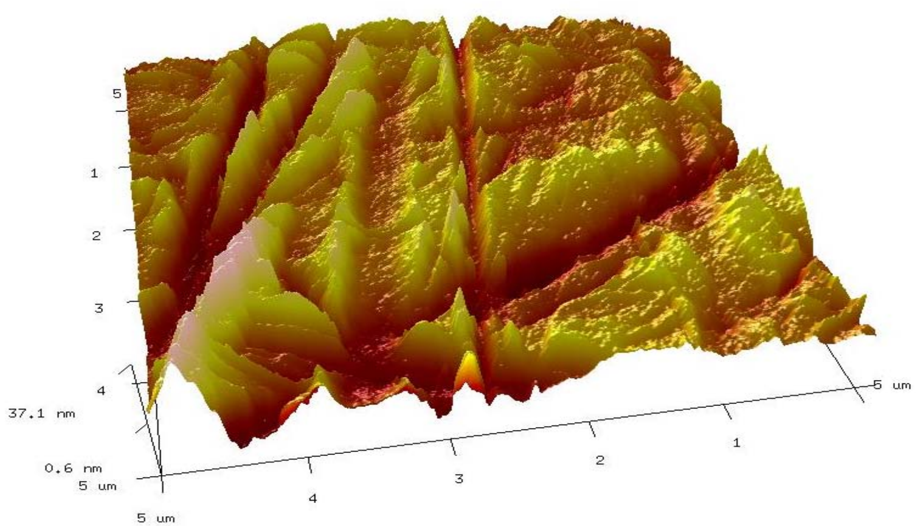


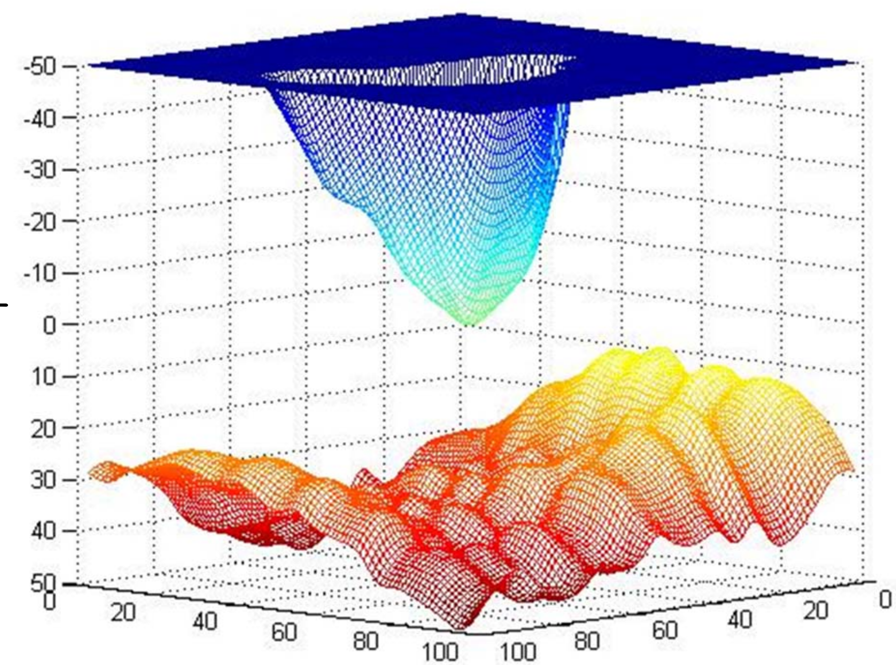
Accounting for Surface Roughness

Topographical Map of Mounted Particle

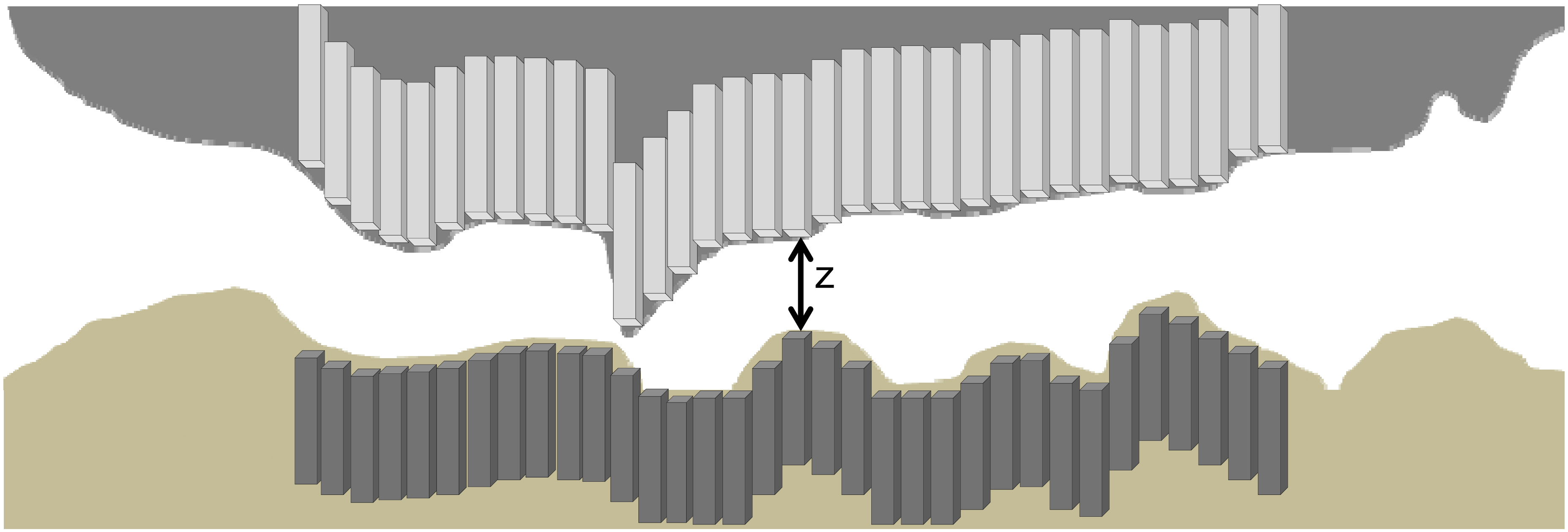


Topographical Map of Substrate





Modeling Adhesion of Rough Surfaces



$$F_{plates}(z) = -\frac{A}{6\pi z^3} \times Area \longrightarrow F_{total} = -\sum_{i}^{n_x}\sum_{j}^{n_y}\frac{A}{6\pi z_{ij}^3} \times Area_{ij}$$

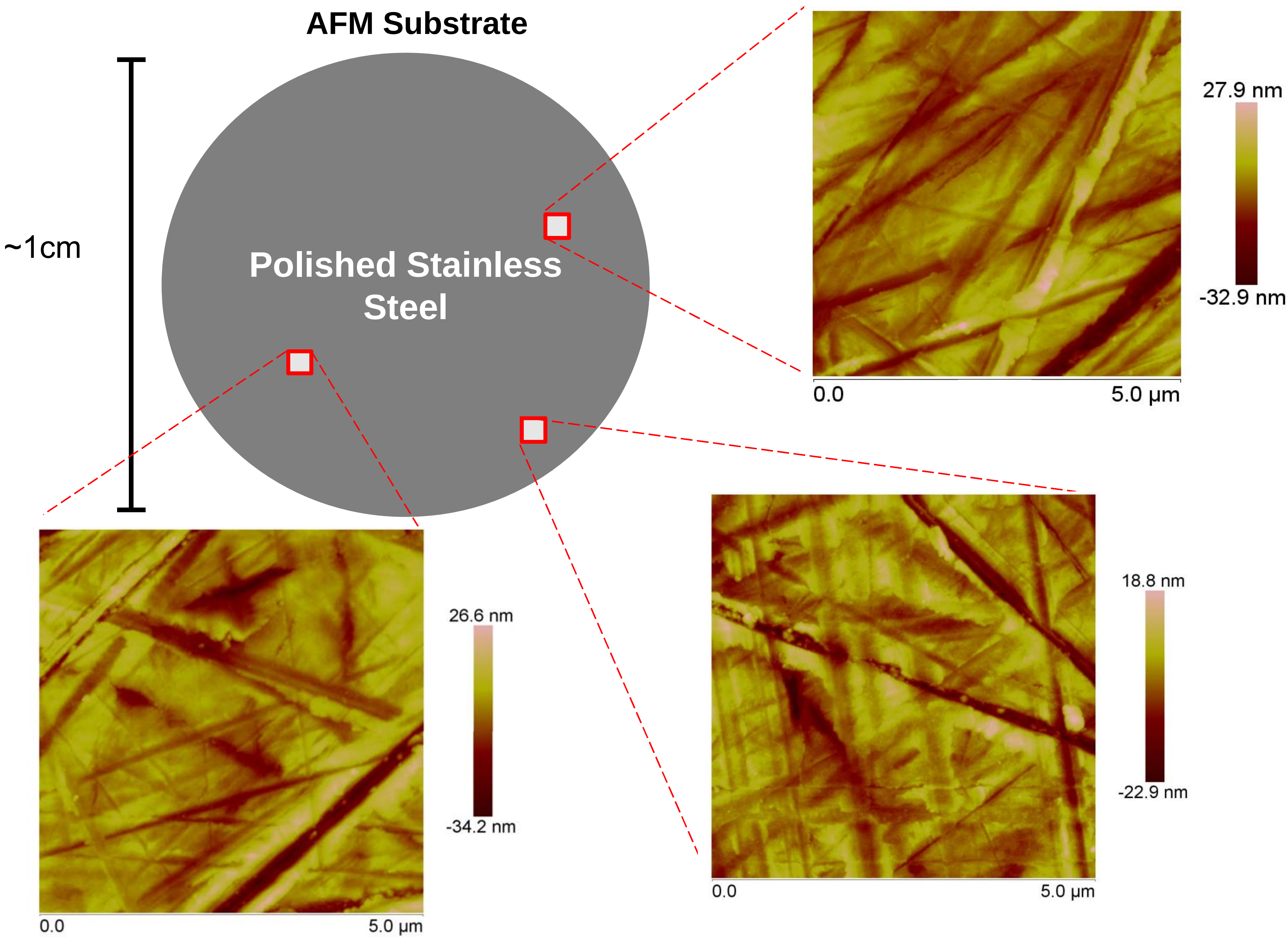
Statistical Considerations

~15cm

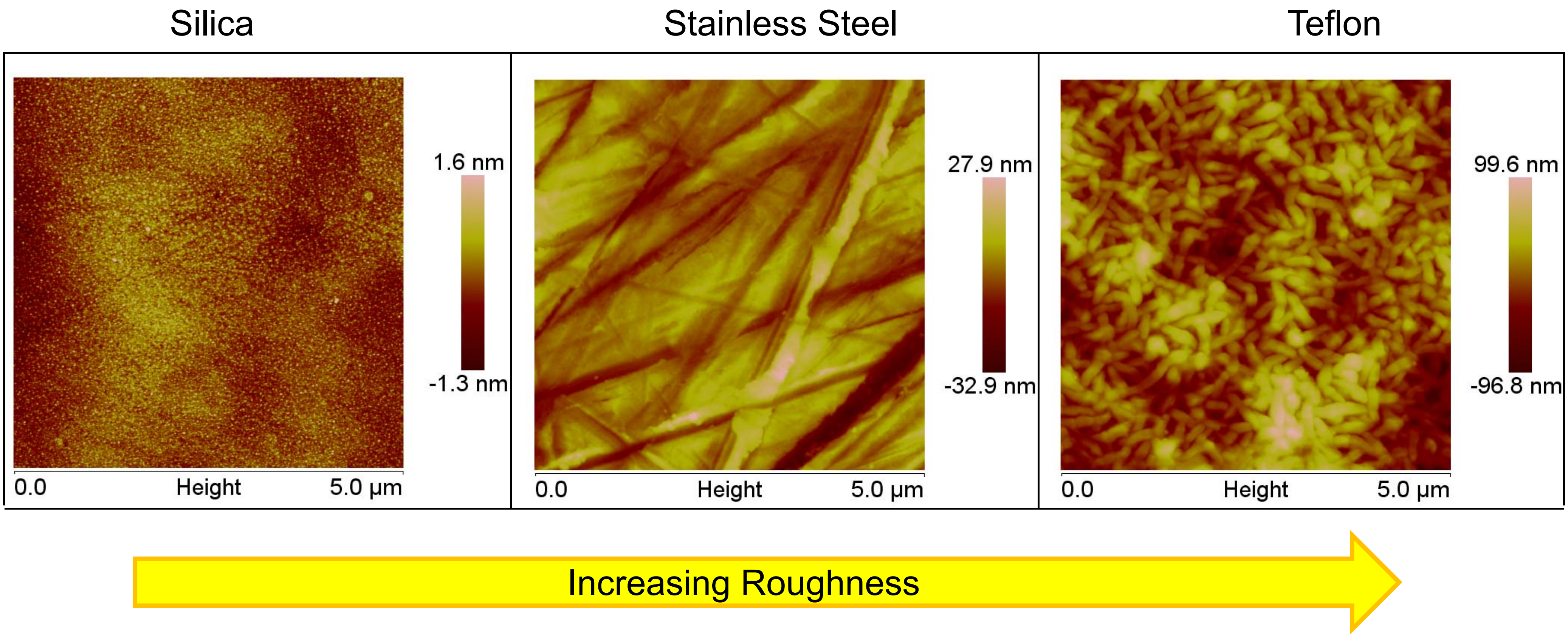
~12cm

~30cm

Statistical Considerations



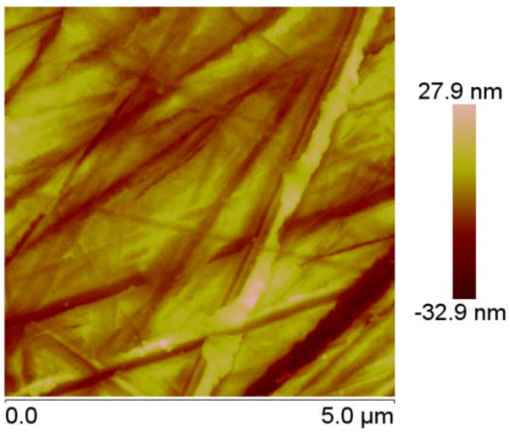
Substrates Considered



Substrate	RMS	Pk-to-Pk
Silica	0.63 ± 0.2 nm	12.8 ± 7.9 nm
Stainless Steel	7.4 ± 1.9 nm	65.9 ± 17.9 nm
Teflon	24.3 ± 5.8 nm	181.2 ± 52.7 nm

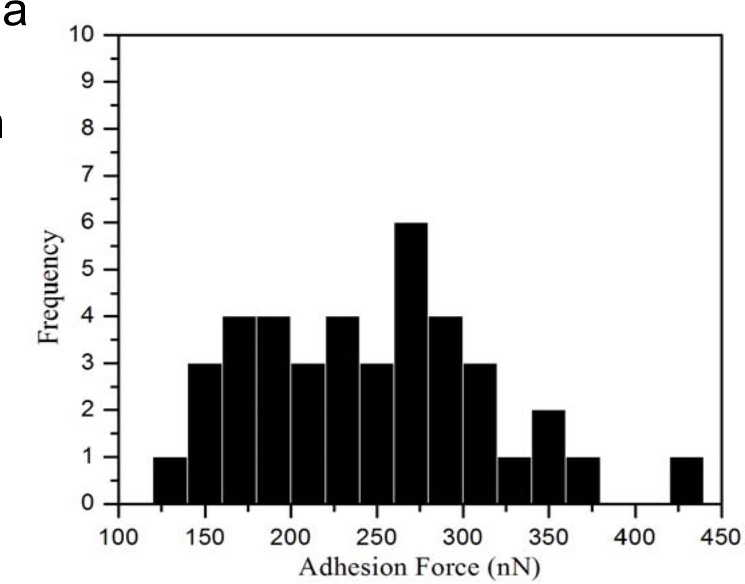
Bootstrap Method

1) Gather AFM Scans (40 locations)

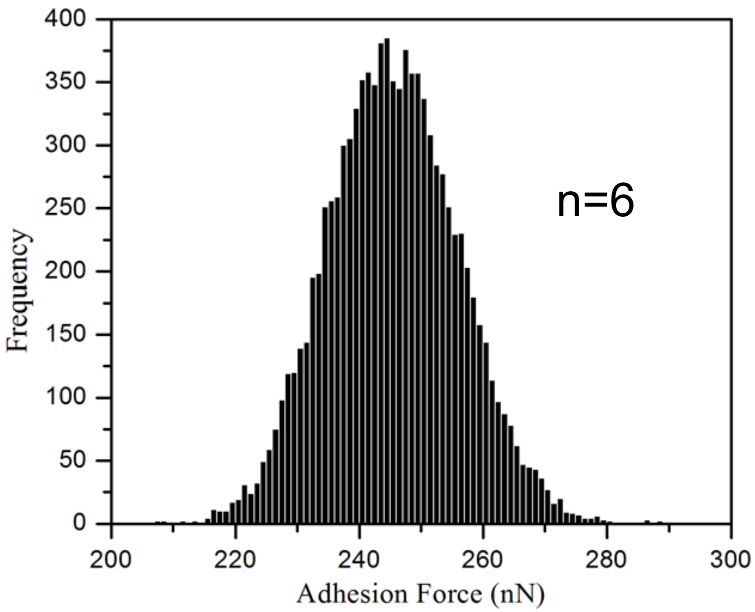


Simulate 10,000 contacts between a particle and each location

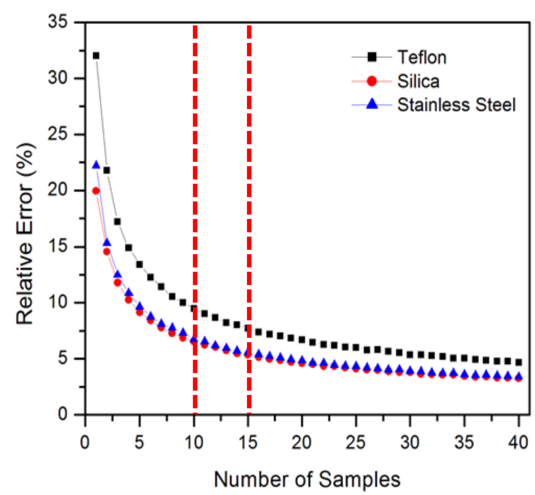
2) Create Parent Distribution (n = 40)



3) Create Bootstrap Distributions



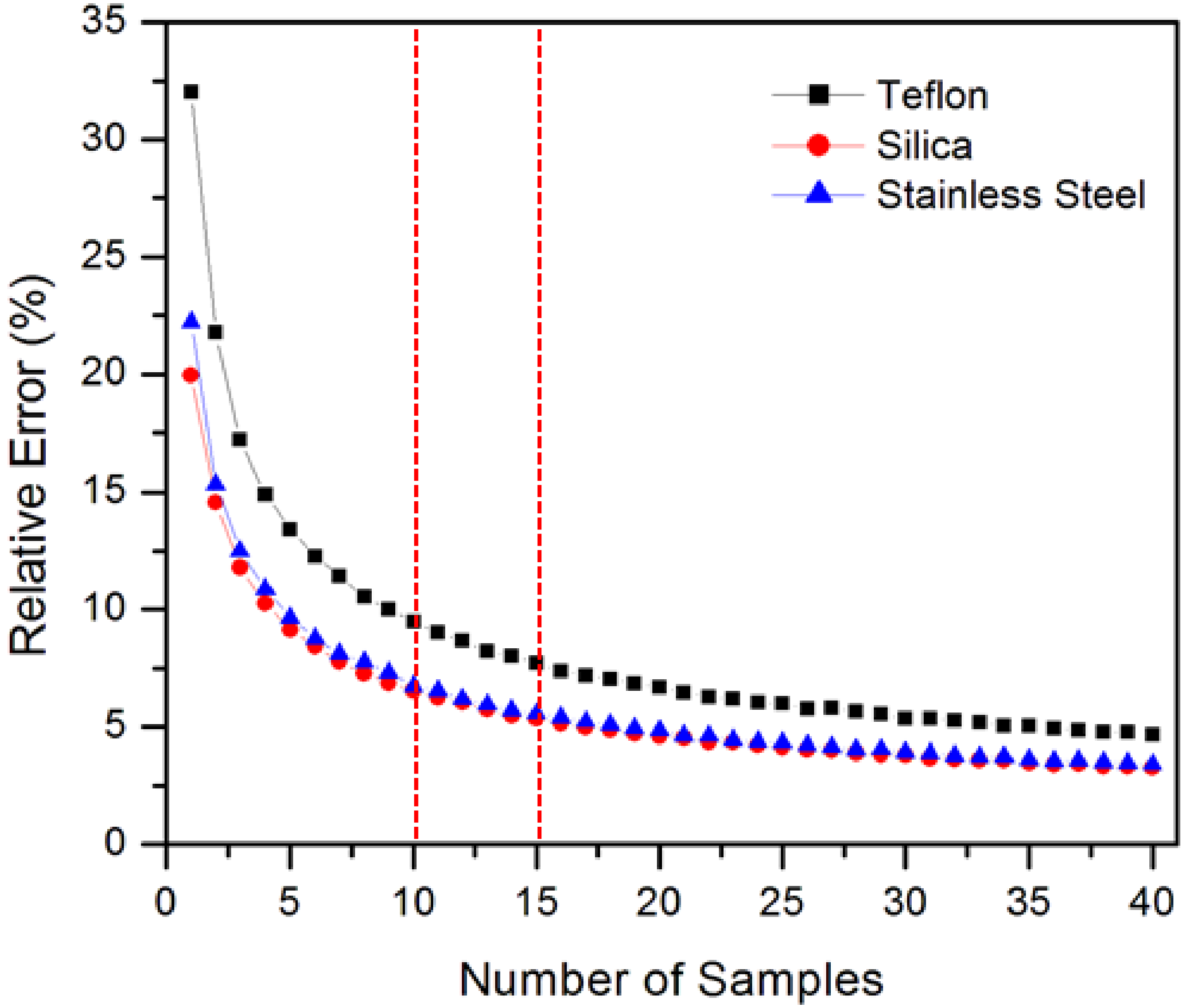
4) Repeat for samples sizes (1≤n≤40)



Statistical Results

Determine optimized number of samples required to fully characterize a substrate

$$RE = \frac{1}{k}\sum_{i=1}^{k}\left|\frac{\bar{x} - \bar{x}_i}{\bar{x}}\right|$$



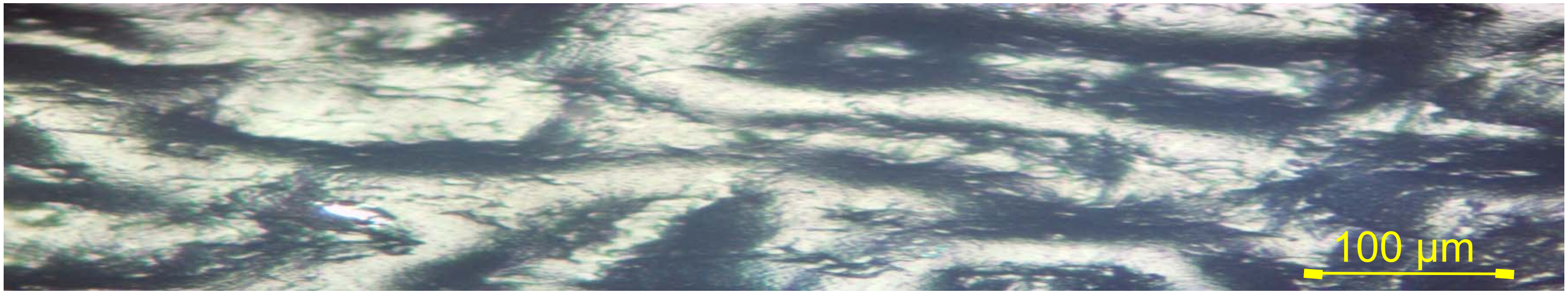
Trace Explosives Application

Surfaces of Interest

Substrate Models

ABS Plastic
- µm-smooth
- µm-rough

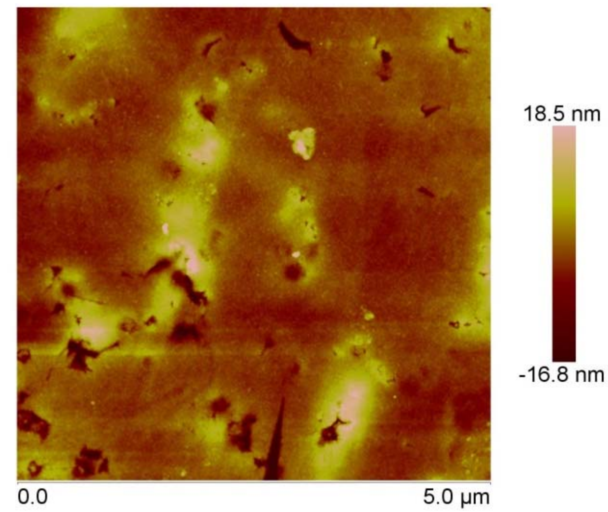
Aluminum
- Paint-coated
- With native oxide



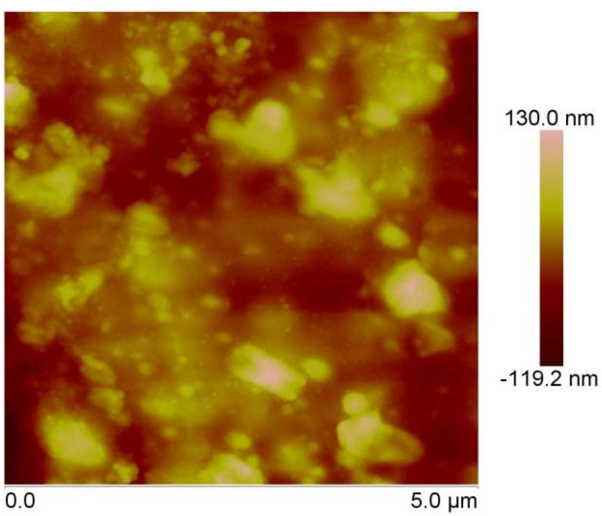
Substrate Roughness Characteristics

Substrate	RMS	Pk-to-Pk
ABS-smooth	66.8 ± 29.9 nm	459.8 ± 134.4 nm
ABS-rough	38.1 ± 20.2 nm	288.6 ± 129.8 nm
Aluminum (native oxide)	60.8 ± 13.1 nm	359.1 ± 120.3 nm
Aluminum (paint-coated)	3.6 ± 0.6 nm	72.6 ± 27.9 nm

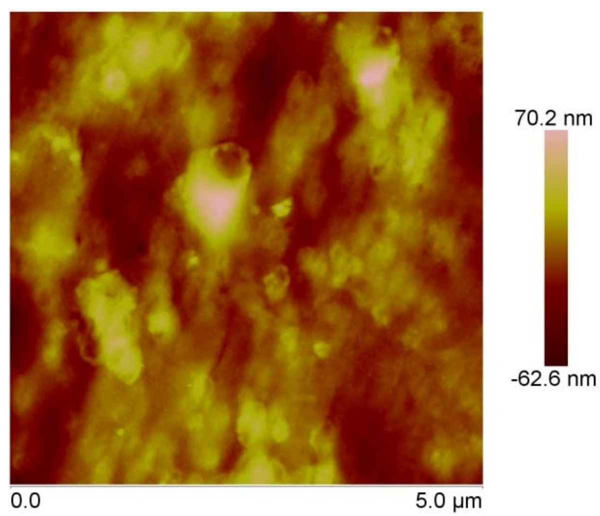
Aluminum
(paint-coated)



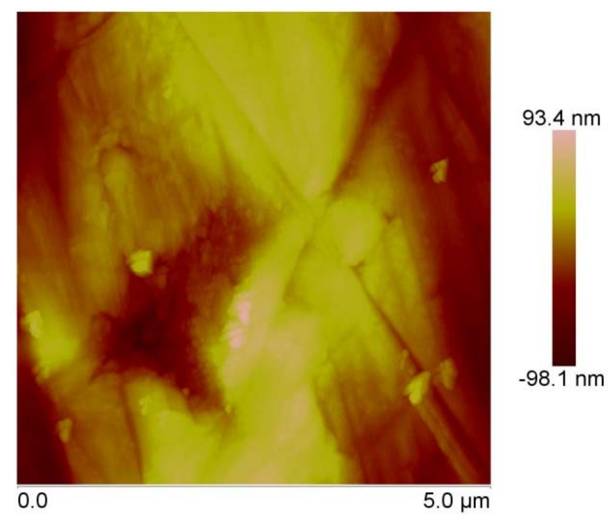
ABS-smooth



ABS-rough



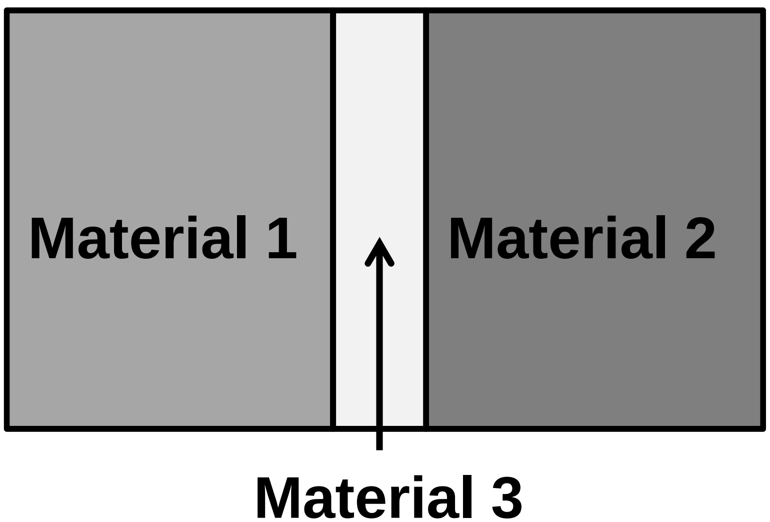
Aluminum
(native oxide)



Hamaker Constant Estimation – Simulator

$$F_{plates}(z) = -\frac{\boldsymbol{A}}{6\pi z^3} \times [Area]$$

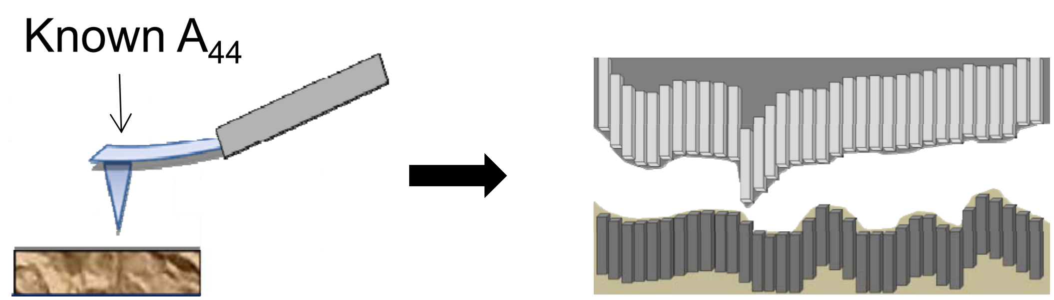
$\boldsymbol{A_{132}}$: The Hamaker constant between materials 1 and 2 interacting through medium 3

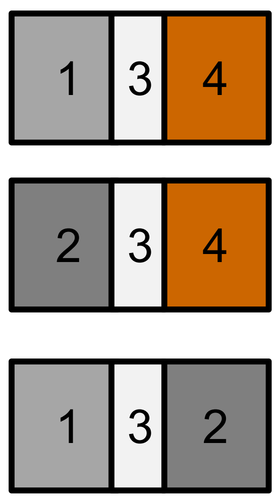


Averaging Approximation

$$A_{132} \approx \left(\sqrt{A_{11}} - \sqrt{A_{33}}\right)\left(\sqrt{A_{22}} - \sqrt{A_{33}}\right)$$

Estimate $\boldsymbol{A_{132}}$ using silicon nitride tip experiments and contact simulator





Step 1. Estimate A_{134} (simulator)

Step 2. Approximate A_{11}

Step 3. Estimate A_{234} (simulator)

Step 4. Approximate A_{22}

Step 5. Predict A_{132}

Hamaker Constant Estimation – Surface Tension

$$W = \frac{-A_{11}}{12\pi D^2}$$

Interaction energy between two planar surfaces (W), Hamaker constant (A), separation distance between the two surfaces (D)

$$W = -2\gamma$$

The total interaction energy is twice the surface energy (γ)

$$A_{11} = 24\pi D^2 \gamma$$

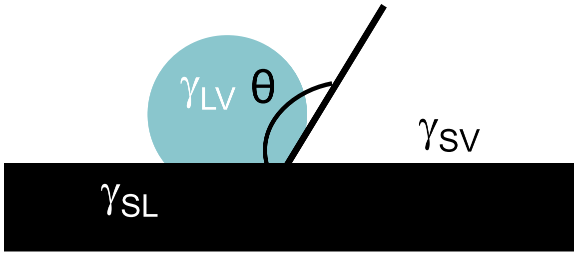
Solve for the Hamaker constant

$$D = D_0 \approx 0.165\, nm$$

Assume the closest separation distance is ~ 0.165 nm

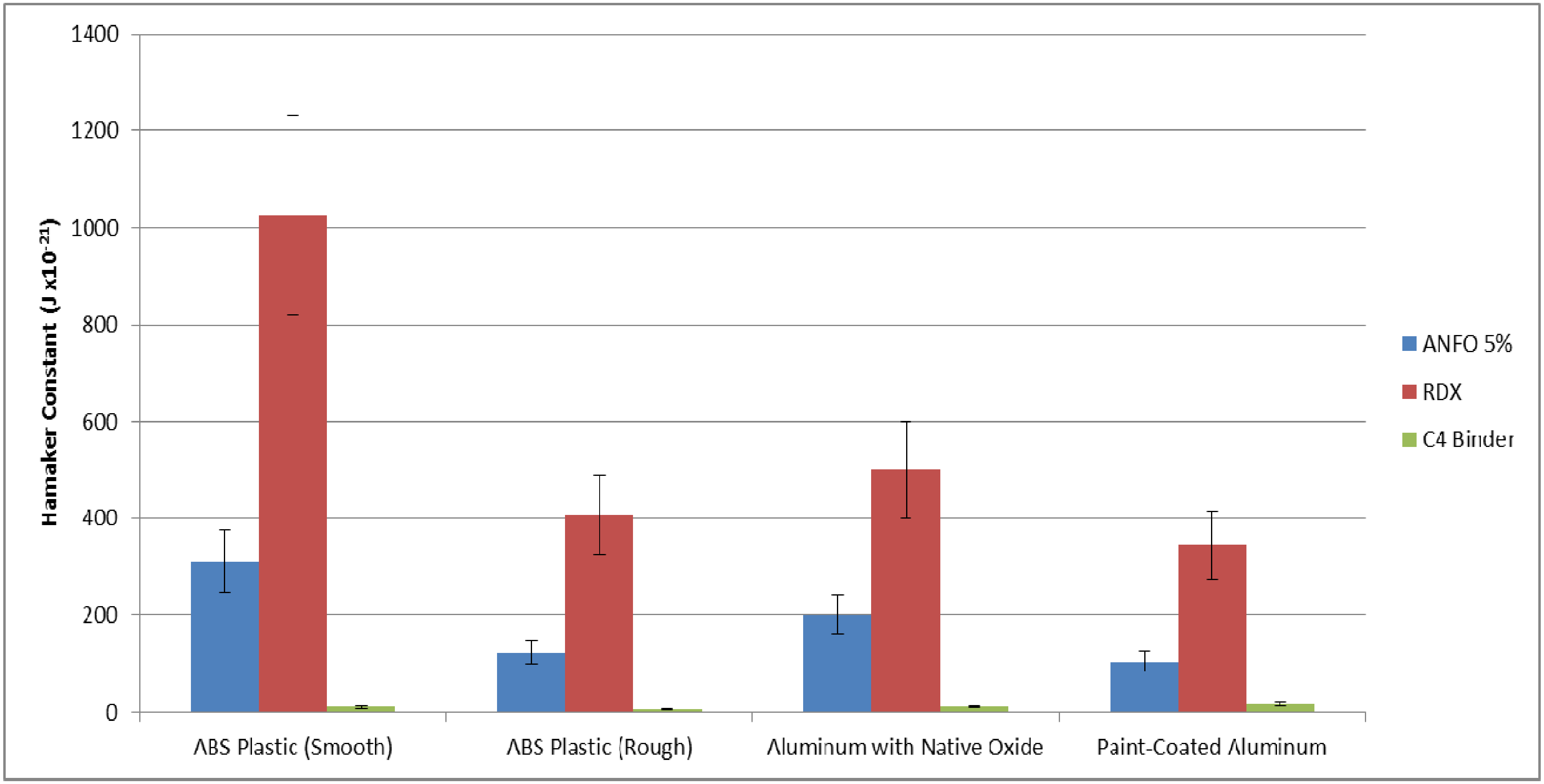
$$\boxed{A_{11} \approx 2.1 \times 10^{-21} \gamma}$$

A (J) estimated from γ (mJ m^{-2})



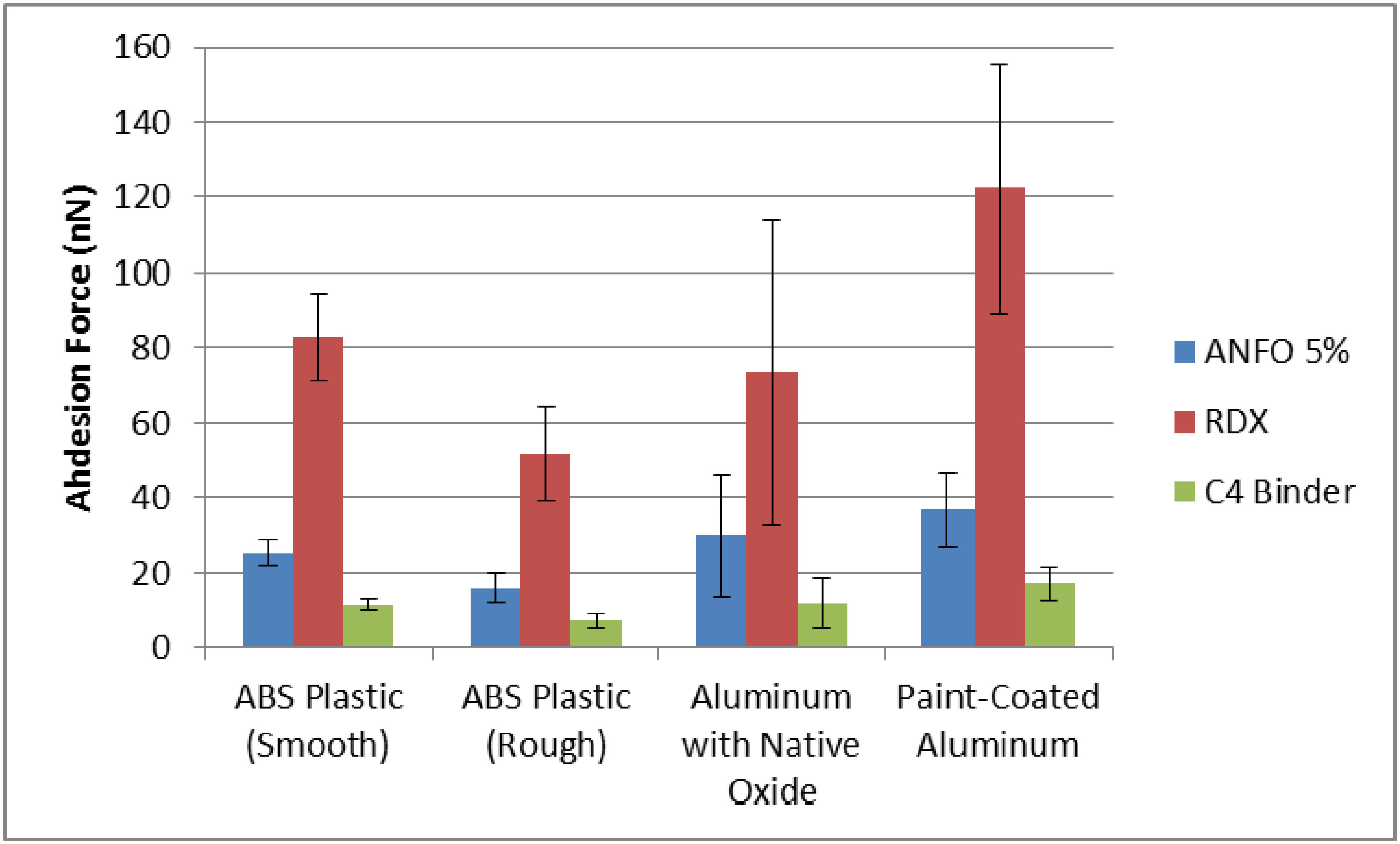
Hamaker Constants

Hamaker constants calculated from self-self interactions

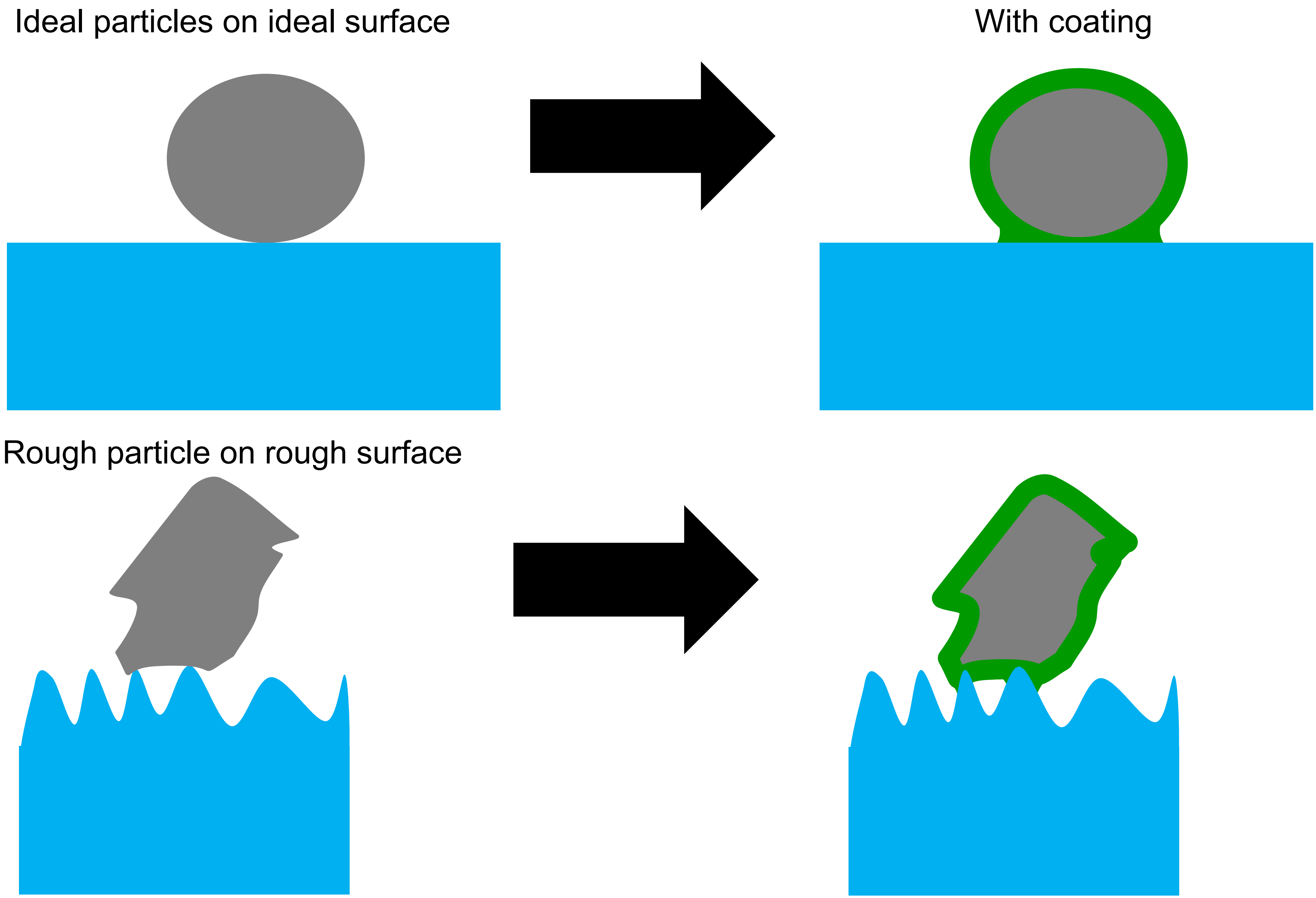


Adhesion Force Predictions

Preliminary results based on 1200 simulated contacts between substrates and 5μm particle

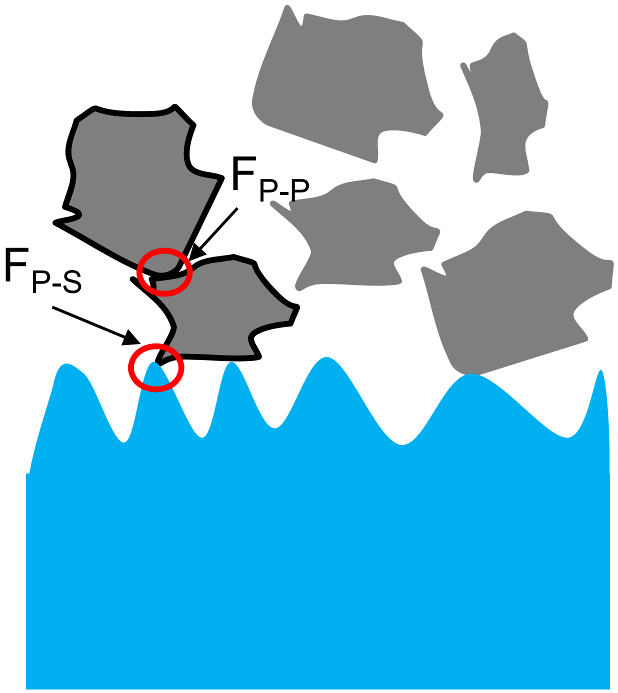


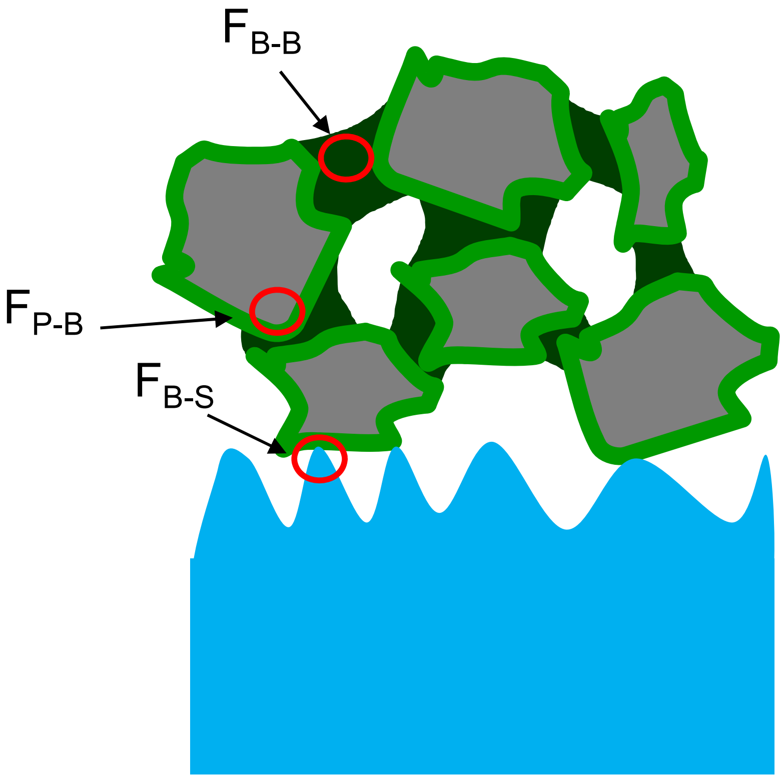
Future Work


Ideal particles on ideal surface
With coating
Rough particle on rough surface

Future Work

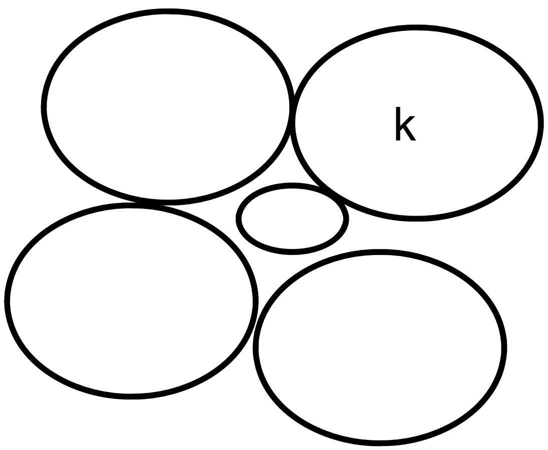
Interactions between the binder, particles, and surface

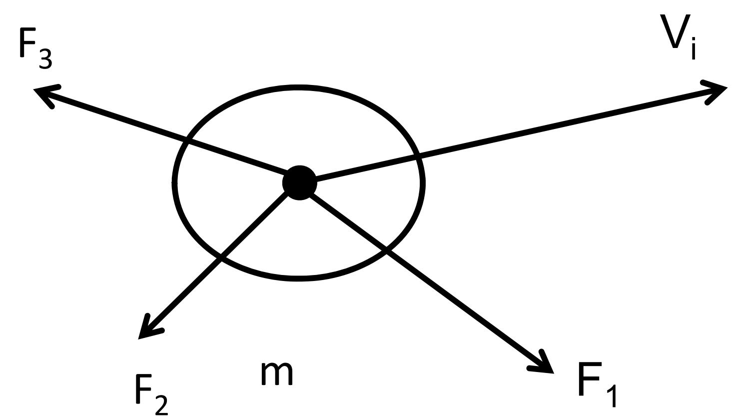




Future Work

Discrete Element Method (DEM)





$$m\ddot{\mathbf{x}}_i = \sum_{j \neq i} \mathbf{f}_{j \to i}$$

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  - Dec. 2015
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Top: Leonid Miroshnik, Sean Fronczak, Jenny Laster, Darby Hoss, Andrew Parker
Bottom: Aaron Harrison, Caitlin Schram, Myles Thomas, Melissa Sweat, Jordan Thorpe

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