

# Awareness and Localization of Explosives-Related Threats (ALERT) *A Department of Homeland Security Center of Excellence*

## *Understanding Contact-Based Sampling for Explosives Detection*

Steve Beaudoin, School of Chemical Engineering, Purdue University



# ALERT

AWARENESS AND LOCALIZATION  
OF EXPLOSIVES-RELATED THREATS

This material is based upon work supported by the U.S. Department of Homeland Security, Science and Technology Directorate, under Award 2010-ST-108-LR0003. The views and conclusions contained in this document are those of the authors and should not be interpreted as necessarily representing the official policies, either expressed or implied of the U.S. Department of Homeland Security.



# Conclusions

- **Fundamental science and engineering understanding can improve the effectiveness of swabs for contact-based sampling**
- **It is possible to understand quantitatively phenomena that control explosives residue adhesion to substrates and swabs**
  - Humidity
  - Composition
  - Deformation
  - Topography
  - Size
  - Shape



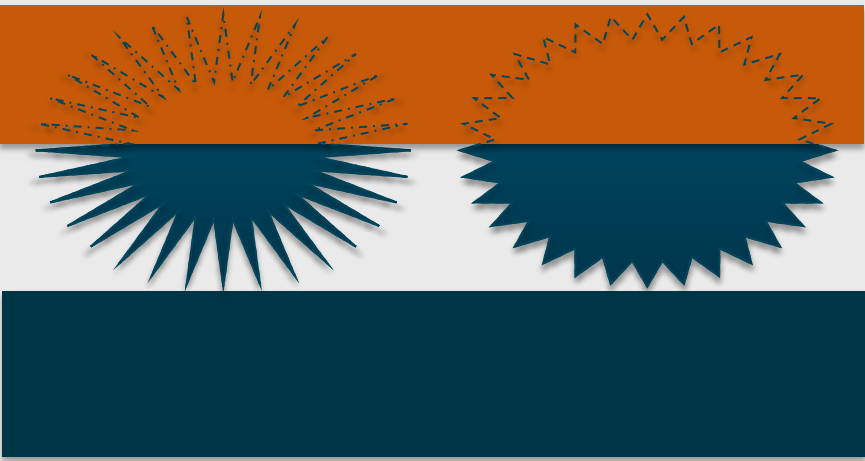
# Research Goals

- Understand adhesion between explosives residues and swabs or substrates
- Use understanding to help guide development of improved swabbing methods/materials
- Parameters considered
  - Residue composition
    - Composites, pure explosives
  - Substrate composition
    - 6 representative surfaces provided by DHS
  - Swab composition
    - 4 common swab types provided by DHS
  - Ambient conditions
    - Primarily relative humidity (RH)



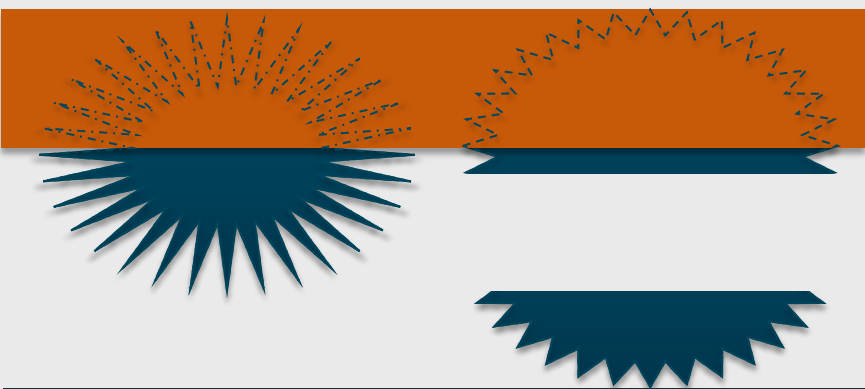
# Fundamentals – Explosives Particle Adhesion

- Mass density within ~25 nm of point of contact controls adhesion
  - Higher mass density = higher adhesion
- Adhesion may be controlled by particle or surface



Low mass density near contact

High mass density near contact

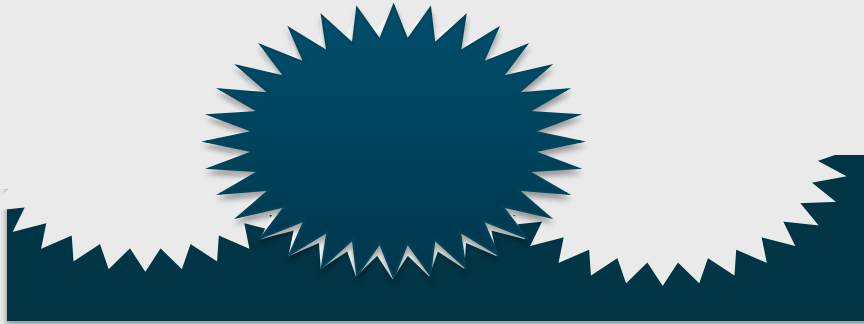


Adhesive failure

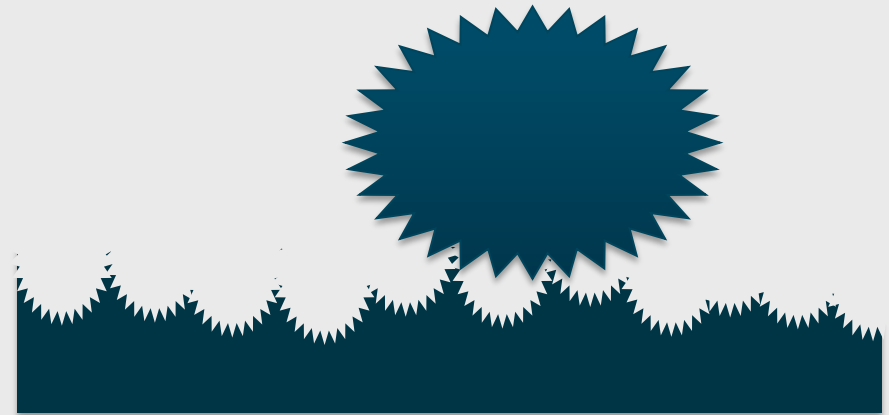
Cohesive failure

# Fundamentals – Explosives Particle Adhesion

- Adhesion may be controlled by particle or surface



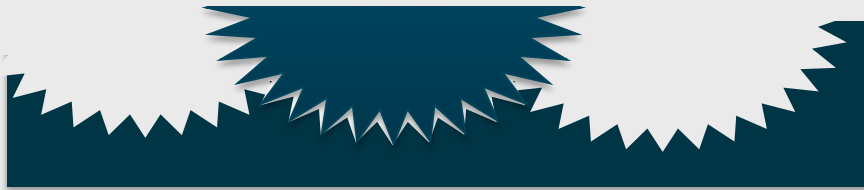
High mass density near contact



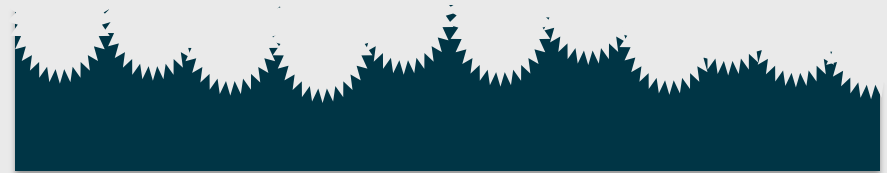
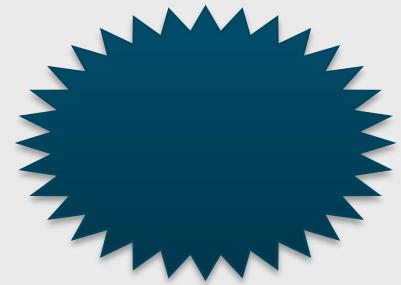
Low mass density near contact

# Fundamentals – Explosives Particle Adhesion

- Adhesion may be controlled by particle or surface



Cohesive failure

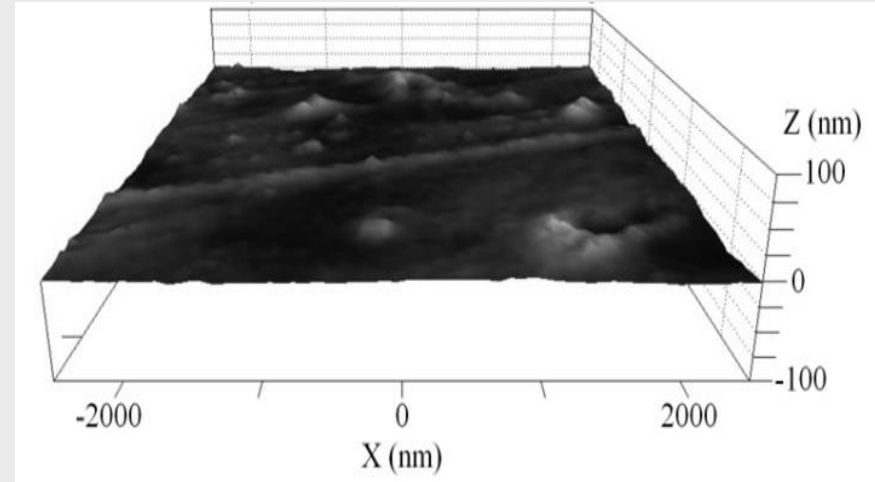


Adhesive failure

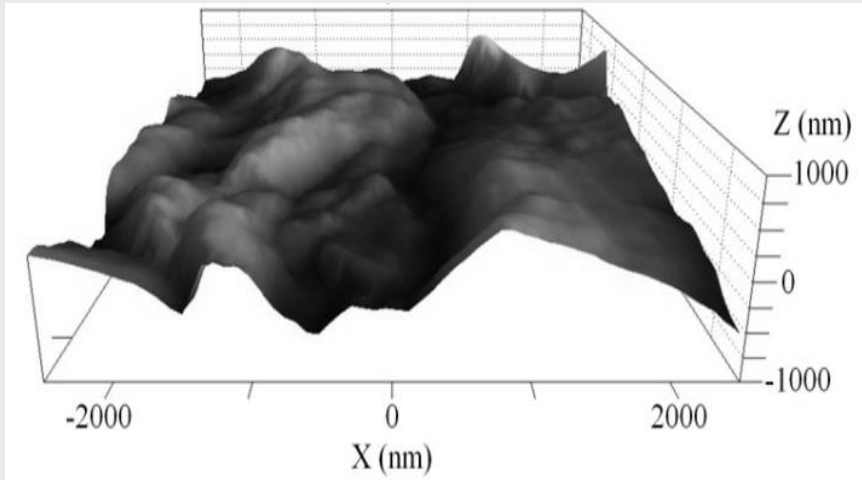


# Adhesion between Explosives and Aluminum

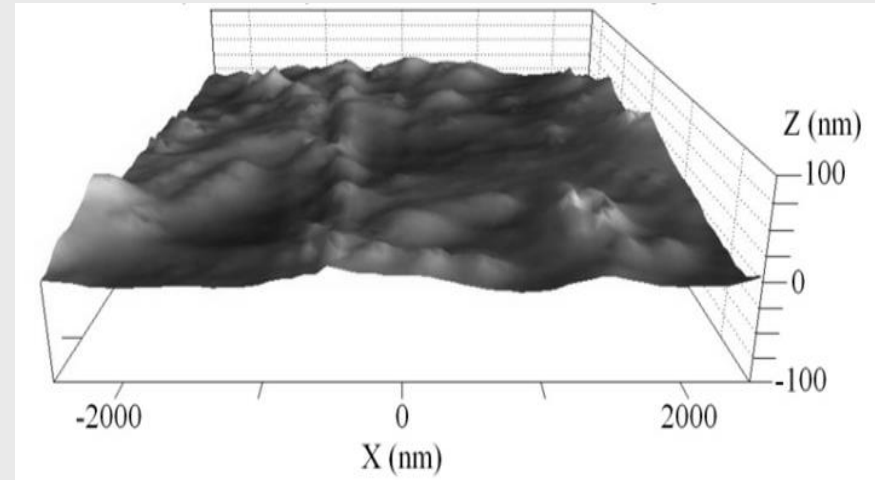
1. Micron-scale particles of PETN, RDX, and TNT mounted on AFM cantilevers
2. AFM used to measure adhesion against aluminum coated with clear-coat (acrylic melamine), white-coat (polyester acrylic melamine), and military coating



Clear-coated aluminum



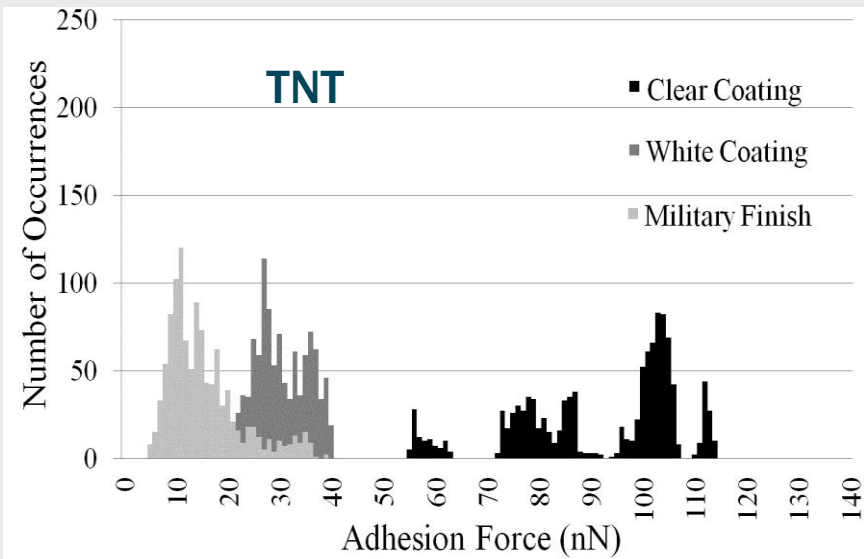
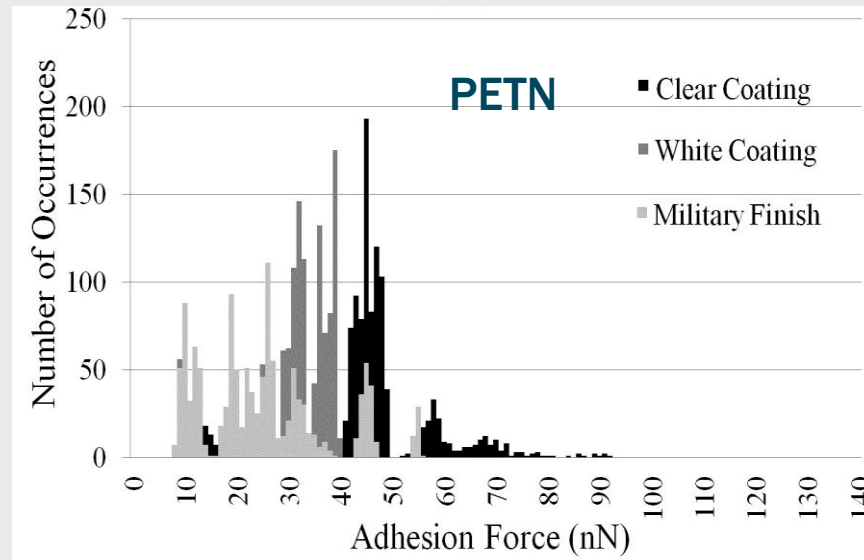
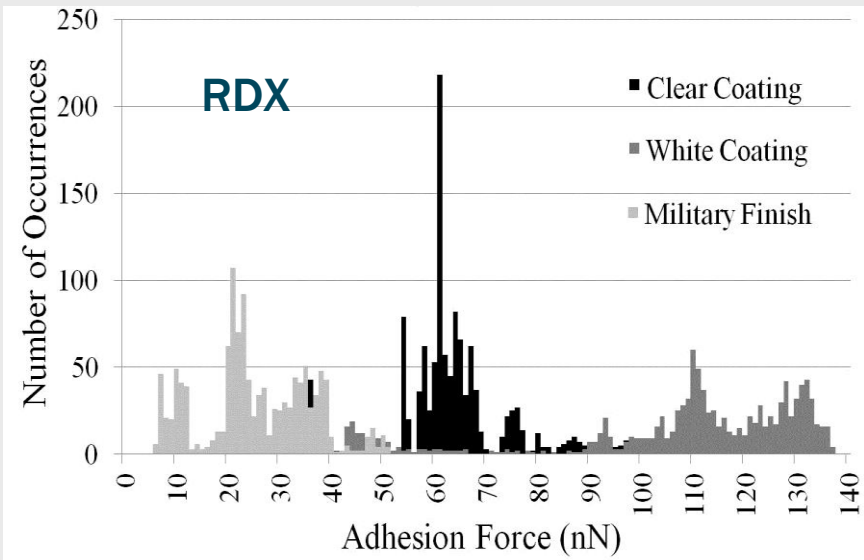
Military coating



White paint with clear-coated aluminum



# Adhesion between Explosives and Aluminum



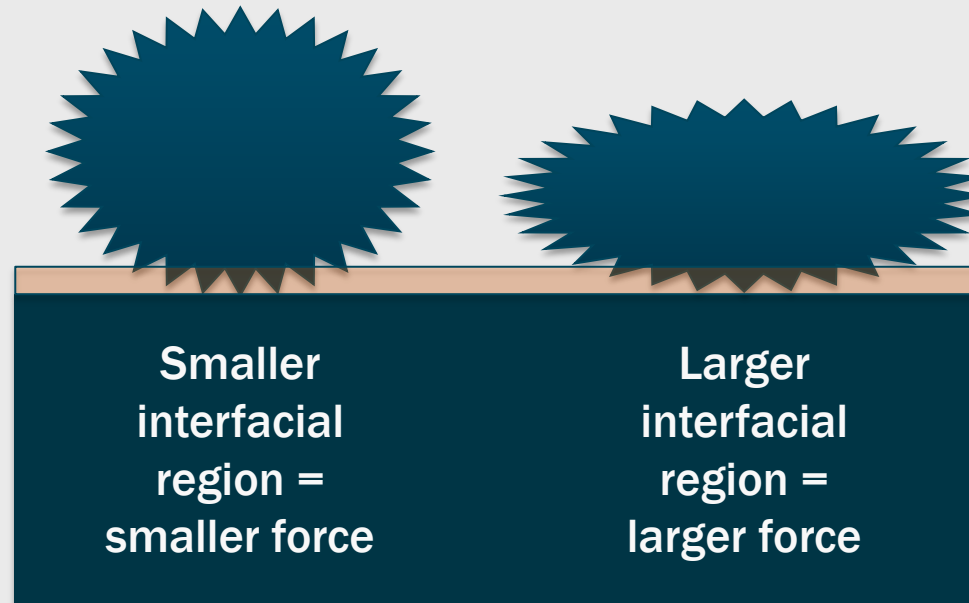
	Force (nN)		
	RDX	PETN	TNT
Clear Coating	63 ± 11	47 ± 12	91 ± 15
White Coating	110 ± 24	32 ± 8	31 ± 5
Military Finish	26 ± 10	26 ± 12	16 ± 7





# Adhesion Influenced by Particle Size

- For a given mass density at interface, increasing the interface size increases the adhesion force



- We eliminate effect of particle size (i.e., to see the intrinsic adhesion force)
  - Evaluate  $\text{force}/(\text{particle radius})$  for spheroids



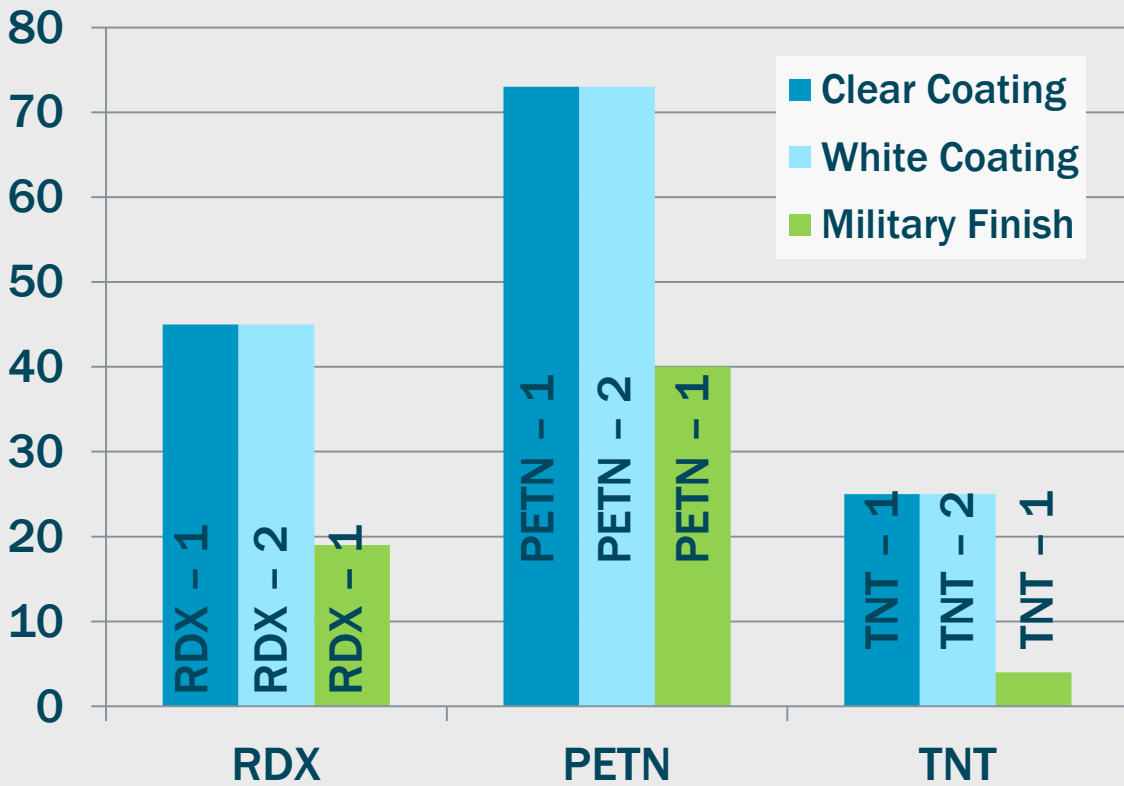
# Normalized Adhesion Forces

- Explosives particles modeled as ‘effective spheroids’ with measured roughness on surface

Surface	Particle	Radius of Curvature of ‘Effective’ Spheroid ( $\mu\text{m}$ )
Clear coated Al	RDX - 1	1.4
	PETN - 1	0.6
	TNT - 1	3.6
White-coated Al	RDX - 2	2.5
	PETN - 2	0.4
	TNT - 2	1.3
Military	RDX - 1	1.4
	PETN - 1	0.6
	TNT - 1	3.6



# Normalized Adhesion Forces



Particle	R.O.C. Ratio (ROC 1)/(ROC 2)	Length Scale
RDX	0.6	0.5 to 3.5 $\mu\text{m}$
PETN	1.5	
TNT	2.8	

- Clear-coat and White-coat
  - Characteristics of particle surface control the interaction
  - Particles very rough on nano-scale
- Military finish
  - Topography (micron-scale) of the military finish controls the interaction



# Describing Roughness Effects

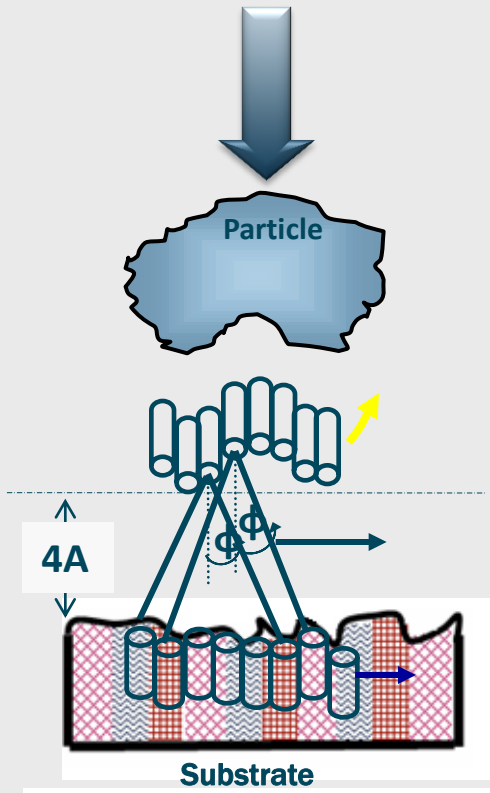
**Model Inputs**  
Surface Morphology  
Material properties

**Computation**  
vdW Force

**Model Prediction**  
Distribution of  
adhesion forces

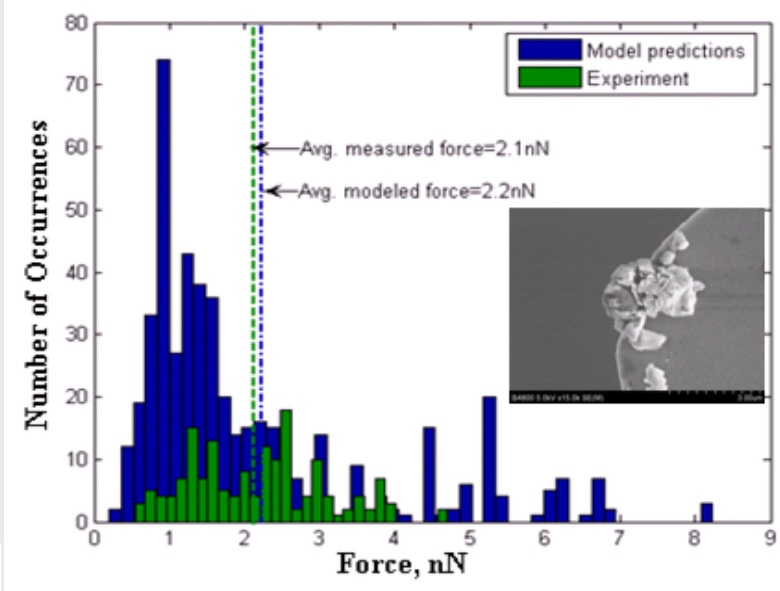
**Geometry**

**Surface Roughness**



$$F_{1j} = C \frac{\partial}{\partial D} \iiint dV_j \iiint \frac{dV_1}{r^{16}}$$

Silicon nitride particle (~3 $\mu$ m) on TaO<sub>x</sub>N<sub>y</sub> in DI water



$F_{,av-Measured}$ : 2.1 nN;  $F_{,av-Predicted}$ : 2.2 nN

- Measured forces in range of model prediction in nearly all cases



# Describing Roughness Effects

- Classical models for van der Waals forces between a cylinder and a plate

$$F_{vdW} = -\frac{A_{132}R^2}{6D^3}$$

- $A_{132}$  = Hamaker constant (fcn of composition of materials and medium)
  - R = cylinder radius
  - D = cylinder-plate separation distance
- In Beaudoin model, when roughness added to equivalent spheroids, Hamaker constant is adjusted to predict distributions

	$A_c^{eff} \times 10^{21}$ (J)		
	RDX	PETN	TNT
Clear Coating	400	300	225
White Coating	425	300	225
Military Finish	800	800	450

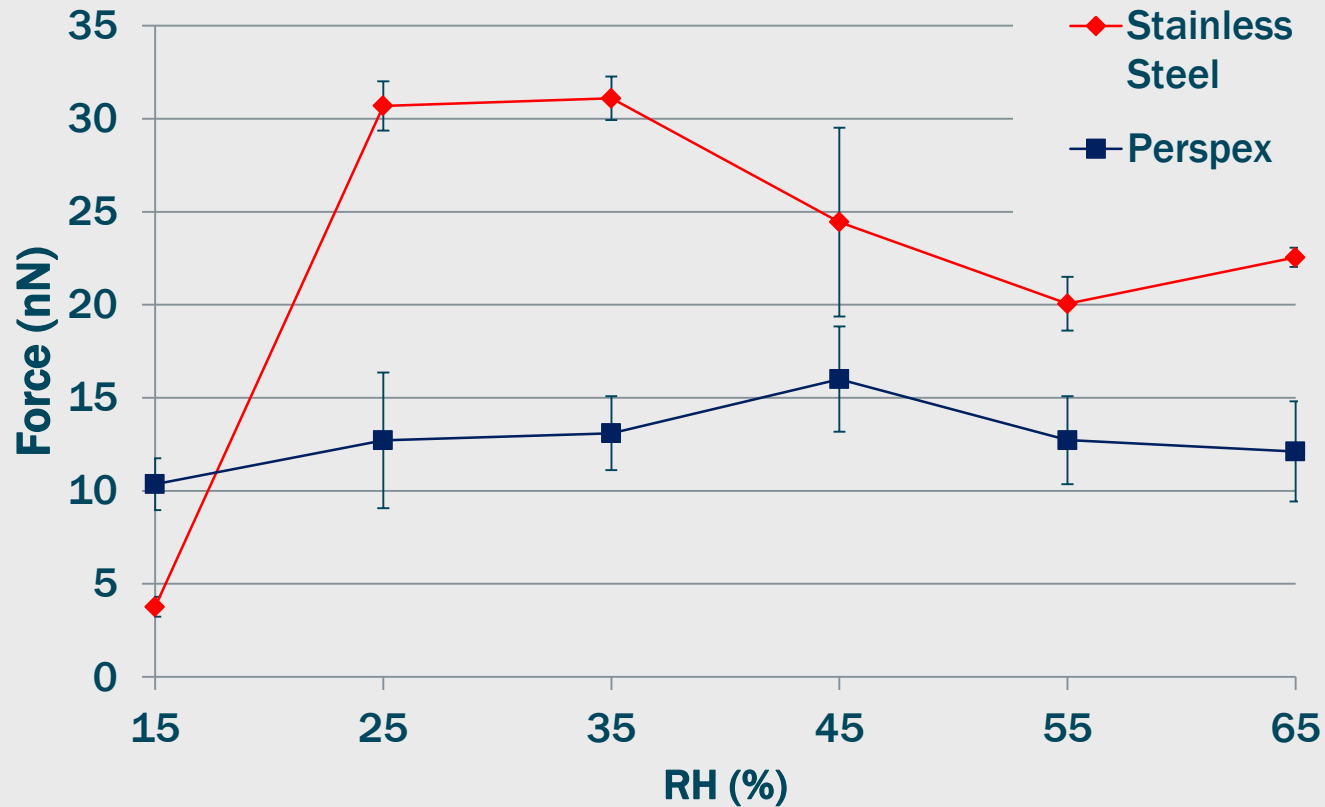
Clear and white coatings have similar composition effects

When present, military finish topography dominates interactions



# Effect of Humidity on Adhesion

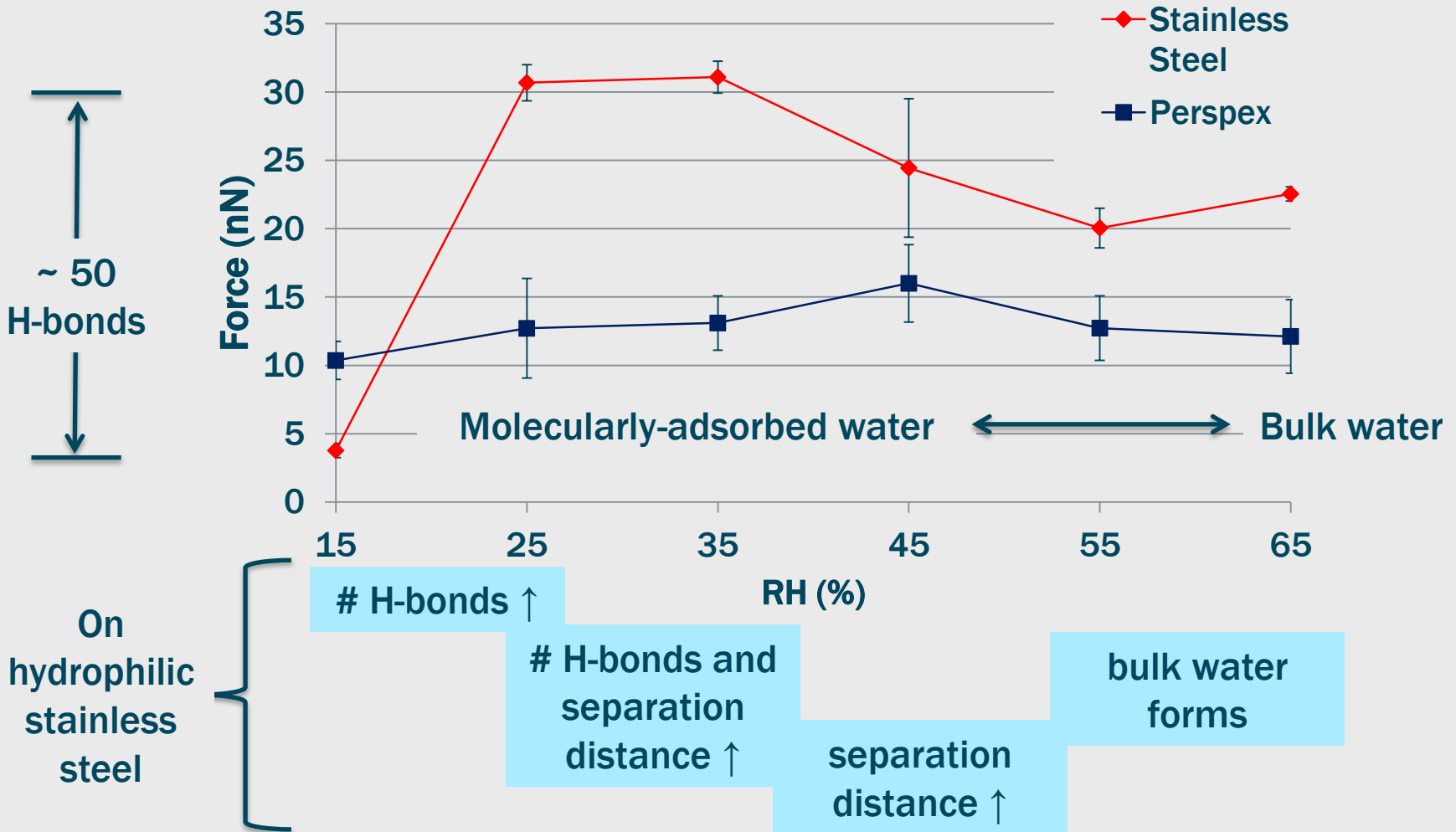
Measured adhesion between silicon nitride cantilever and surfaces





# Effect of Humidity on Adhesion

- At most RH levels, 'bulk' water on a surface does not exist
- Water at lower RH (< 50 - 55%) levels is molecularly-adsorbed, sub-continuum
  - No surface tension, but does support H-bonding



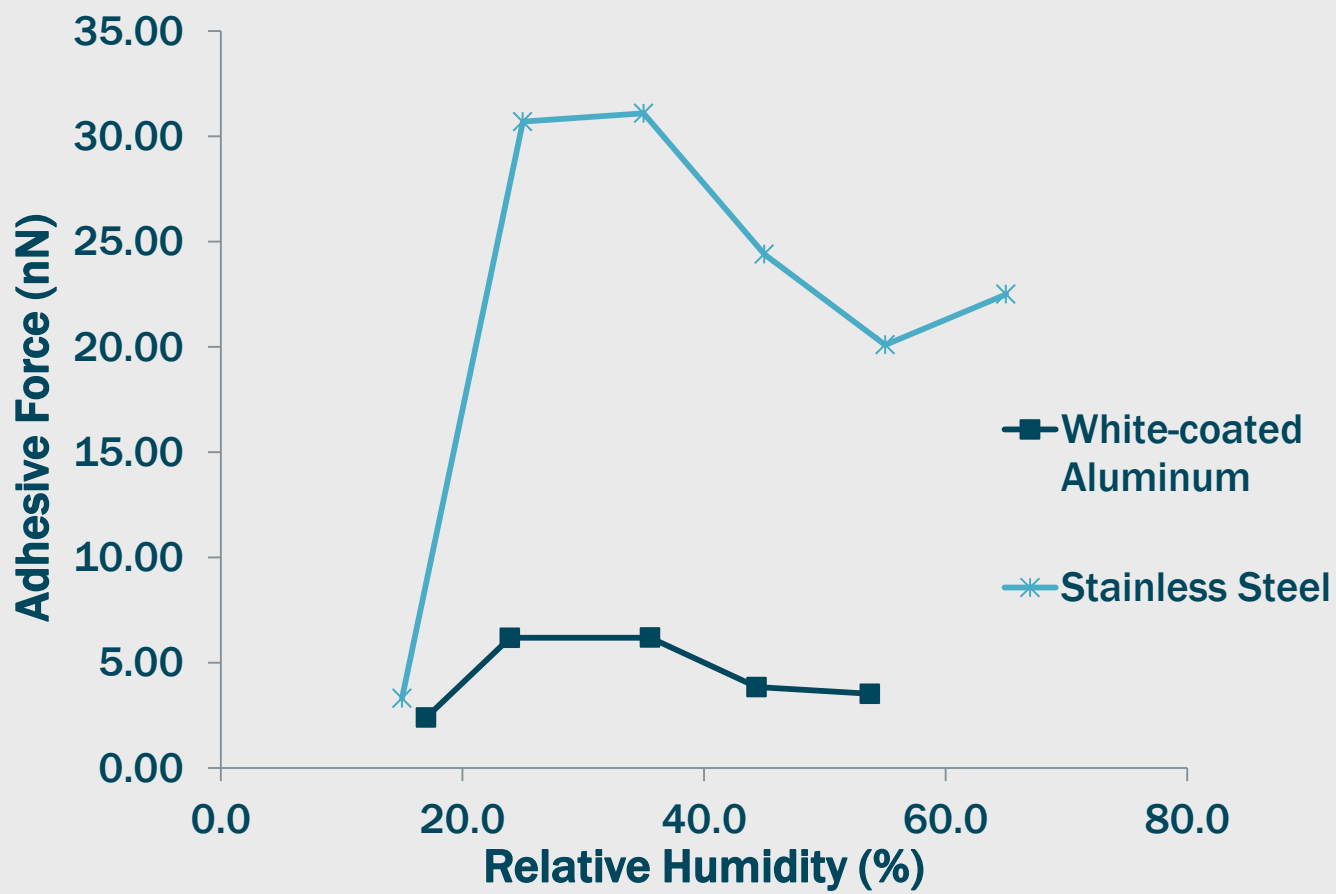


# Effect of Humidity on Adhesion

- Metal, hydrophilic surfaces show adhesivity increase as RH rises below 35%
  - Due to adsorbed molecular water
- Show a decrease from ~35 - ~55%
  - Due to water forming a barrier to close contact

- Adhesion increases again as RH rises above 55%
  - Due to bulk water drops on surface

For hydrophilic surfaces, one would expect significant changes in adhesion when RH changes at low levels



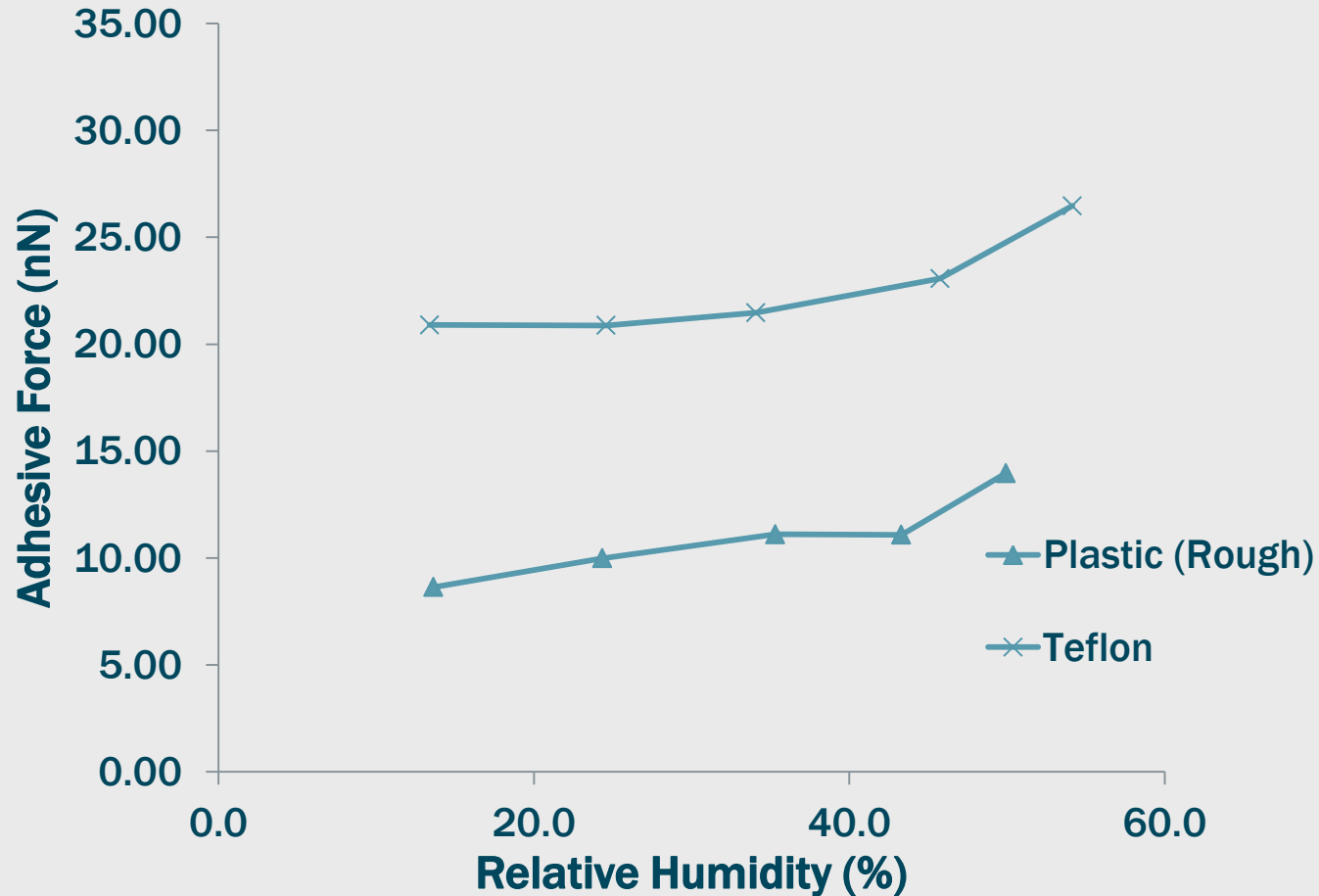




# Effect of Humidity on Adhesion

- Hydrophobic surfaces show minor changes in adhesivity  $RH < \sim 50\%$ 
  - Due to minimal tendency to adsorb molecular water
- Show larger increases above 55%
  - Due to bulk water drops on surface

For hydrophobic surfaces, one would expect insignificant changes in adhesion when RH changes at low levels





# Ongoing Work

- **Extend current studies to describe composite explosive materials**
  - C4, SEMTEX, ANFO
  - Deformation during residue removal key to overall process
- **Develop improved swab materials based on mechanical properties of swabs and residues**



# Acknowledgements

- **U.S. Department of Homeland Security, Science and Technology Directorate sponsored this work under agreement 2010-ST-108-LR0003**