Contact Modeling
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Large-scale MD simulations
Given the surface roughness and chemistry of the PRISM device predict:
- Force-displacement curves for device simulation
- Pull-out force and adhesion energy (stiction)
- History and rate dependent (contact area evolution)
- Possible generation of subsurface defects in metal and dielectric

Stage 1: long-range interactions
- Interaction dominated by attractive van der Waals forces: Hamaker constant

Stage 2: impact
- Elastic constant between asperities
- If: local stress > material hardness → plastic deformation
- Solid bridging can occur
- Defect generation

Stage 3: pull-out
- vdW interactions
- If solid bridging occurs: need to overcome strength of solid bridges

Atomistic metal-dielectric contact
Method & Force Fields

• Size dependence with maximum at around 5 nm
• \( \sigma_{\text{tension}} > \sigma_{\text{contact}} \) as metal-metal contact
• Mass transfer during contact and opening at large contact size
• Linear increase of contact area

Uncertainty Quantification and validation

Mesoscale contact model

PRISM Si3N4 surface topology (AFM)

- Attractive van der Waals interaction:
  \[
  F_{\text{vdW}}(\vec{r}) = -A \sum_{i,j} \frac{\Delta L^2}{6\pi \xi_{ij}^3 + \vec{r}^2}
  \]

- Repulsive contacts (Hertz) – assumes elastic contacts
  Estimate the number of contacts from average curvature of contact region and overlap volume

\[
F_{\text{cont}}(\vec{r}) = N_{\text{cont}} \frac{2}{3} E^* R \delta^3
\]

• Force-distance
• Contact area
• Contact stress

Uncertainty Quantification and validation

UQ with respect to input properties:
- Response surface (A and E*) and surface topology
- Stochastic process