Predictive atomistic modeling in PRISM: Roadmap
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GOAL
Identify, characterize and quantify the fundamental mechanisms that govern the response of the PRISM device

Inform device-level simulations
- Dielectric charging
- Mechanical response
- Solid-fluid interactions

Dielectric charging
Characterize the formation of electrically active defects in dielectric induced by:
- Temperature
- Impact
- Electrical current & electric field

- ReaxFF to predict structures
- Ab initio, density functional theory calculations to compute electronic levels
- Collaborate with P. A. Schultz (Sandia)
- SeqQuest code

Years 2-4

Impact simulations
Large-scale atomistic molecular dynamics simulation
- Surface roughness evolution in multi-contact
- Defect generation during contacts
- Surface-surface interaction
- Role of electric current (local heating)

Years 1-5

Mechanical response of metallic bridge
- Dislocation-based plasticity in Ni
  - Nucleation and propagation
  - Interaction with grain boundaries
  - Deformation in TiO2 film
  - Grain sliding

- Large-scale MD simulations using LAMMPS
  - Year 1: existing state of the art potentials
  - Years 2 on: first principles-based potentials (e.g. charge equilibration)
  - Impact simulations as well as uniaxial tension

Years 1-3

Solid-fluid interaction
Given a distribution of incident momenta characterize the distribution of reflected momenta:

\[ \sigma_i = \frac{E_i - E_r}{E_i - E_s} \]
\[ \alpha_r = \frac{p_r - p_i}{p_i} \]

Fluid FVM models use accommodation coefficients from MD and predict incident distribution

Role of roughness and surface moisture on accommodation coefficients

Years 3

Planned large-scale simulations
- Ni with EAM potential
- SiO2
- 32,000 atoms / processor
- Force cutoff of 4.8 Å
- Steele: 0.117 sec per MD step
- SiCortex: 1.04 sec per MD step

- 9,000 atoms / processor
- Force cutoff of 5.5 & 9.0 Å

- 32,000 atoms / processor
- Force cutoff of 4.8 Å
- Steele: 0.117 sec per MD step
- SiCortex: 1.04 sec per MD step

Planned FY08 simulations
- Size: 131M Ni atoms – Simulation time: 500ps
- Resources: 4096 BGL processors for 45 hours
- Size: 131M Ni atoms + 37M-atom SiO2 – Simulation time: 100ps
- Resources: 4096 BGL processors for 45 hours