LAMMPS User Group Meeting
August 7-8, 2013

PECVD generated Silicon films with kinetic Monte Carlo and LAMMPS molecular dynamics

Dr. Andreas Bick

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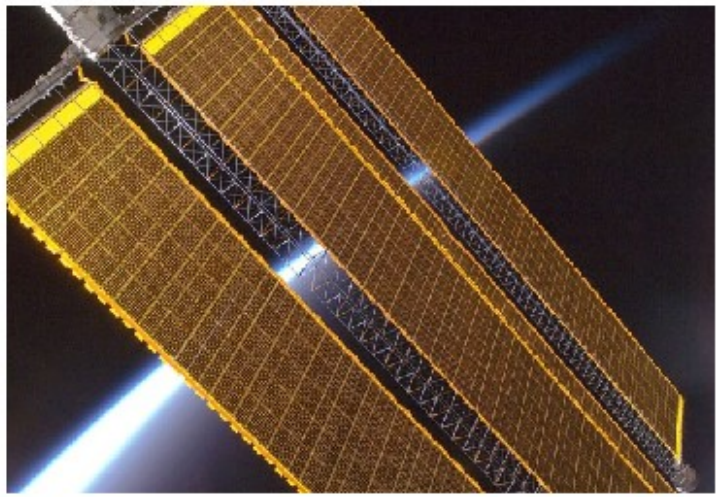
Albuquerque, 2013

Motivation: Silicon is everywhere



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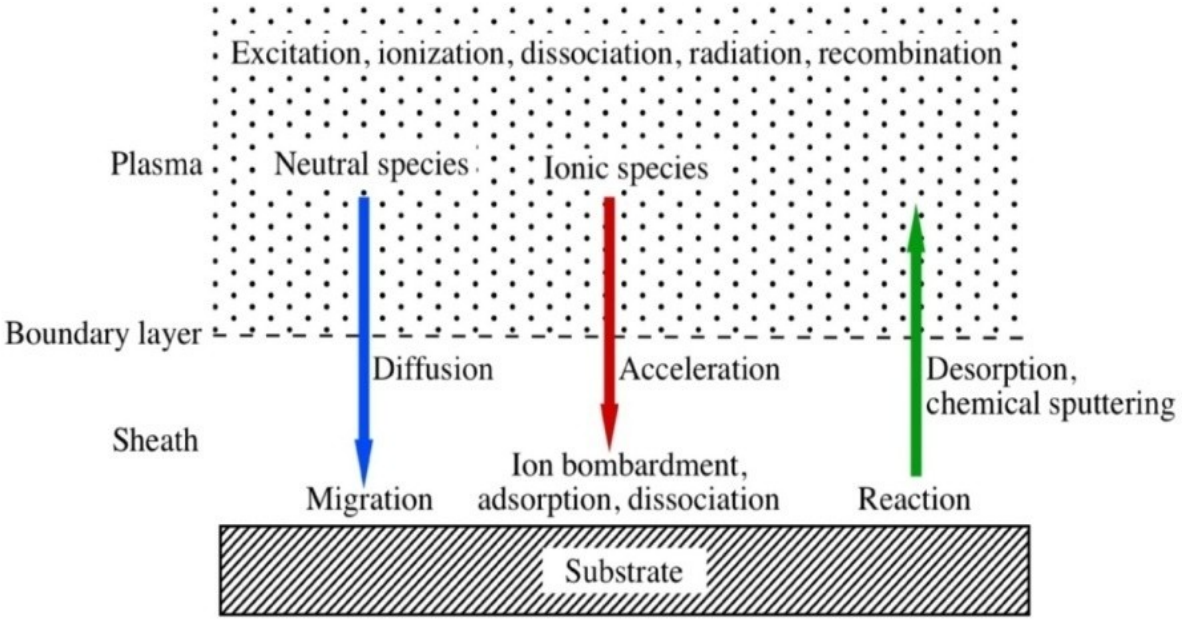
Plasma Enhanced Vapor Deposition

- **Chemical Reaction**
  - SiH_4 -> Si + 2 H_2
  - Deposits thin films from a gas state (vapor) to a solid state on a substrate
  - Used for electronics, optoelectronics and photovoltaic applications
  - Fast deposition at low temperatures
  - Surface interactions and film growth not yet fully understood



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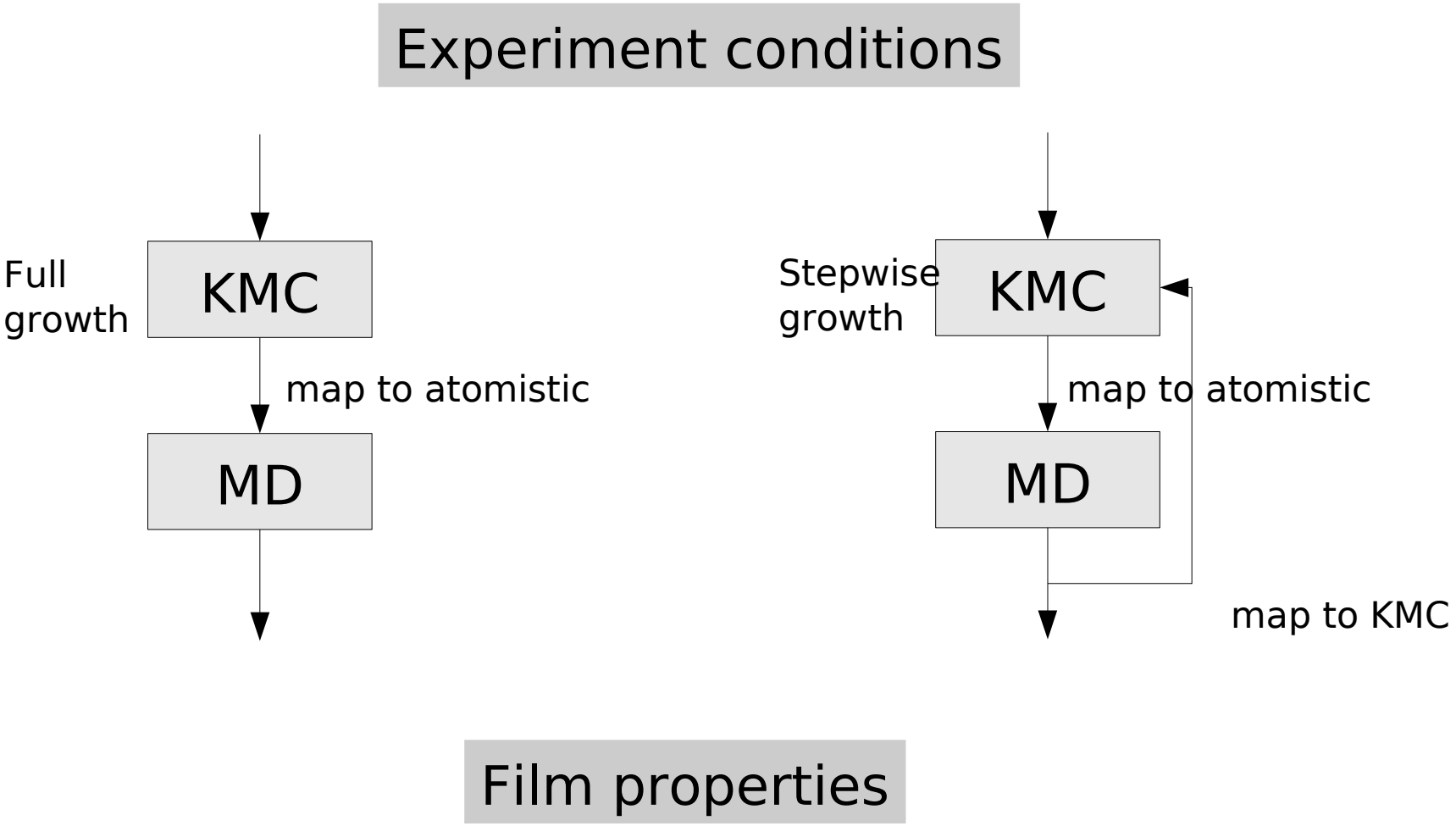
Combine KMC and MD



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Kinetic Monte Carlo(n- fold method)

- **Based on Diamond lattice**
- **Complex chemical reaction involving different radical species**
  - Physisorptions & Chemisorptions of gas phase radicals
  - Bulkilization of Hydrogen passivated Si
  - Subsequent abstraction of surface atoms (Eley-Rideal Hydrogen Abstractions)
  - Surface diffusion of physisorbed radicals
- **Two separate reaction steps (Decoupled diffusion methodology)**
  - Diffusion (Markovian Random Walk)
  - All the other reactions

Kinetic Monte Carlo(n- fold method) II

- At each step a complete list of possible reactions for all surface sites is considered
- Reaction event j is randomly selected according to:

$$R = \sum_{i=1}^{i=M} r_i \qquad \frac{\sum_{i=1}^{i=j-1} r_i}{R} < \xi_1 < \frac{\sum_{i=1}^{i=j} r_i}{R} \quad (1)$$

with the random number chi, the total number of possible reactions per step M and the reaction rate r

- The time increment delta R is calculated as

$$\delta t = -\frac{\ln(\xi_2)}{R} \quad (2)$$

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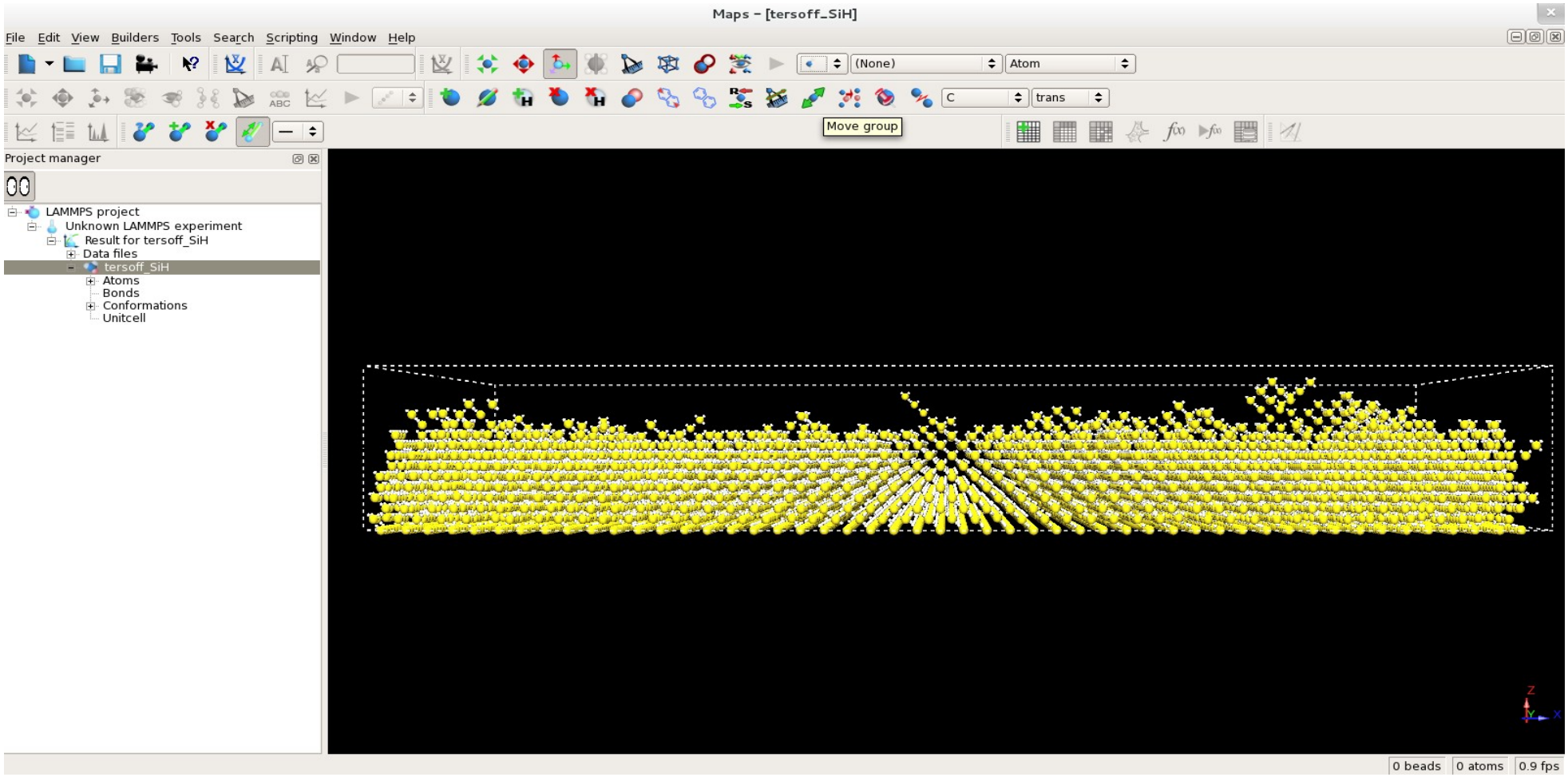
KMC Results:

- **Snapshot of KMC generated surface visualized in MAPS:**



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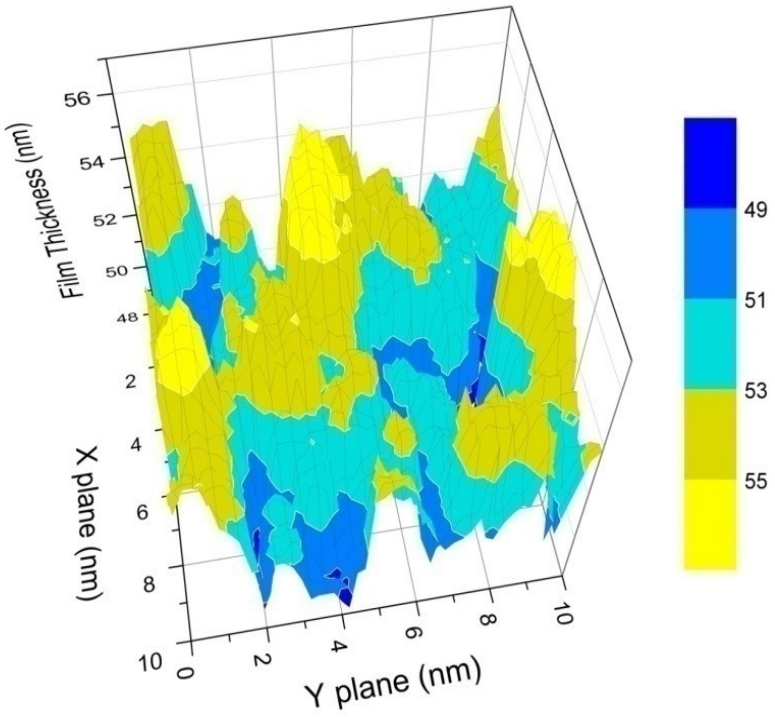
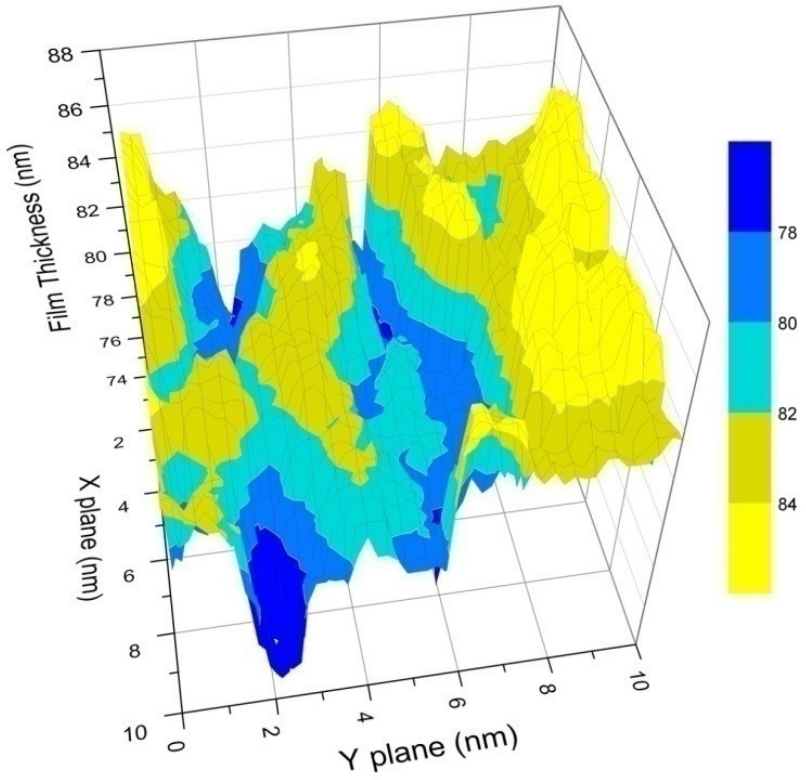
KMC Results:

- **Surface thickness dependent on SiH content:**





5 % SiH

6 % SiH

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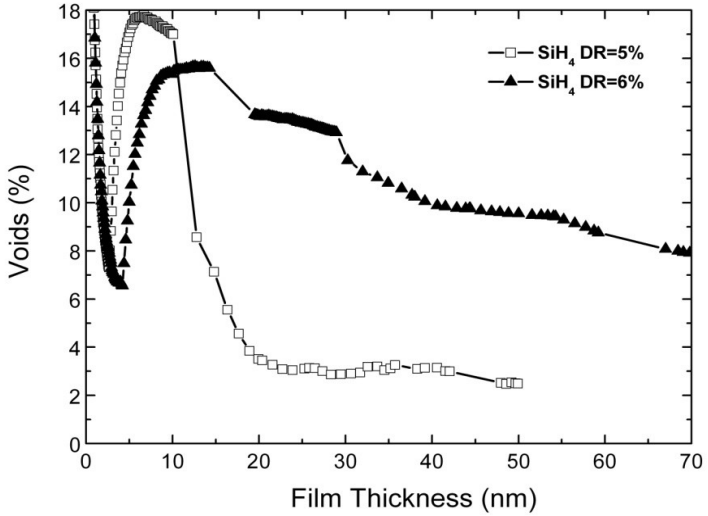
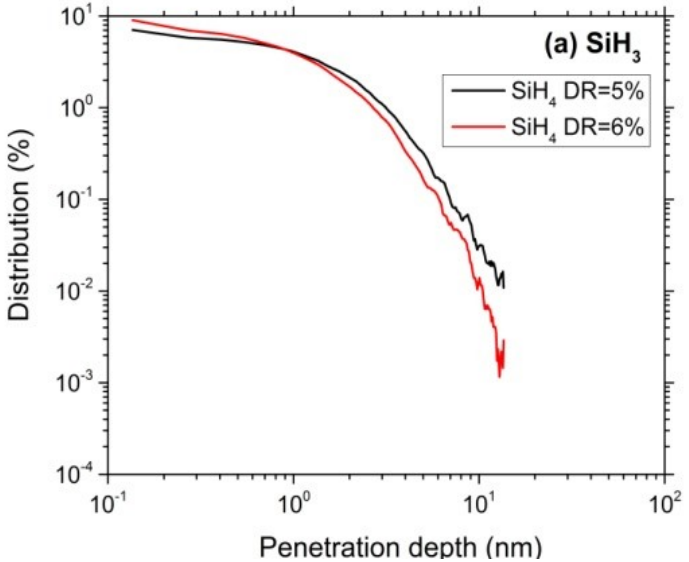
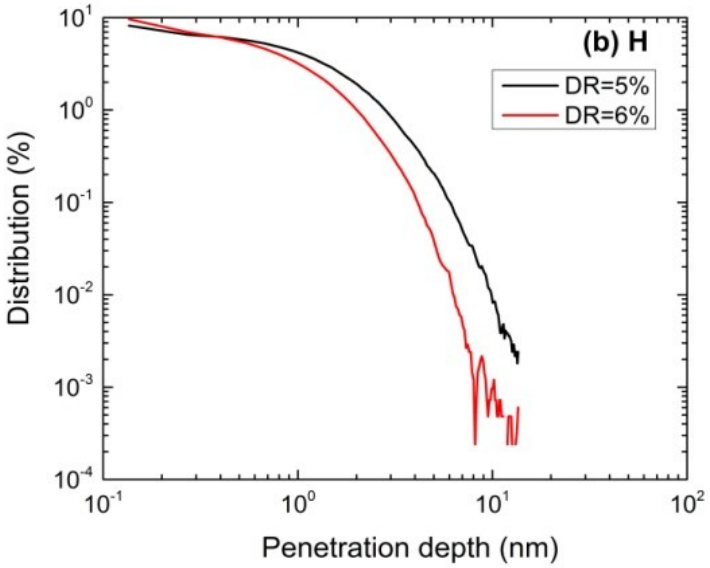
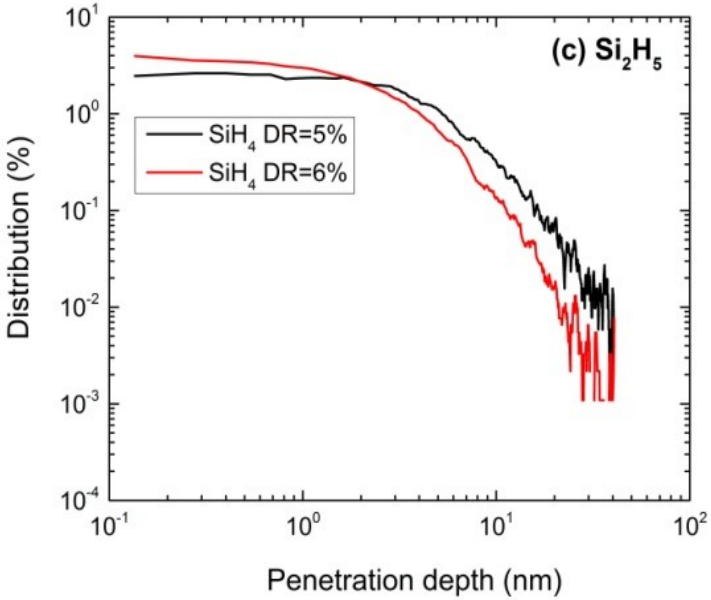
KMC Results: Void distribution









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Molecular Dynamics (LAMMPS)

- **Newton's equation of motion**

$$F = m\,a$$

- **The force can be written as the gradient of the potential energy**

$$F = -\nabla V$$

- **Combine the two equations to get**

$$\frac{dV}{dr} = -m\frac{d^2 r}{dt^2}$$

- **A trajectory is obtained by solving this differential equation**
- **NVT Simulations using the Nose Hover thermostat at 180 K performed for this study**

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Tersoff Potential

- **Bond Order Potential**
- **Strength of a chemical bond depends on the bonding environment, including the number of bonds and possibly also angles and bond length**
- **Exists in several modifications**
- **Implementation in LAMMPS needed modification to the functional form developed by Ohira**

$$V_{ij} = f_C\left(r_{ij}\right)\left[a_{ij} f_R\left(r_{ij}\right) + b_{ij} f_A\left(r_{ij}\right)\right]$$

Where the interaction parameter aij describes the repulsive Si-H interaction

- **Implemented in LAMMPS for this project by Scienomics**

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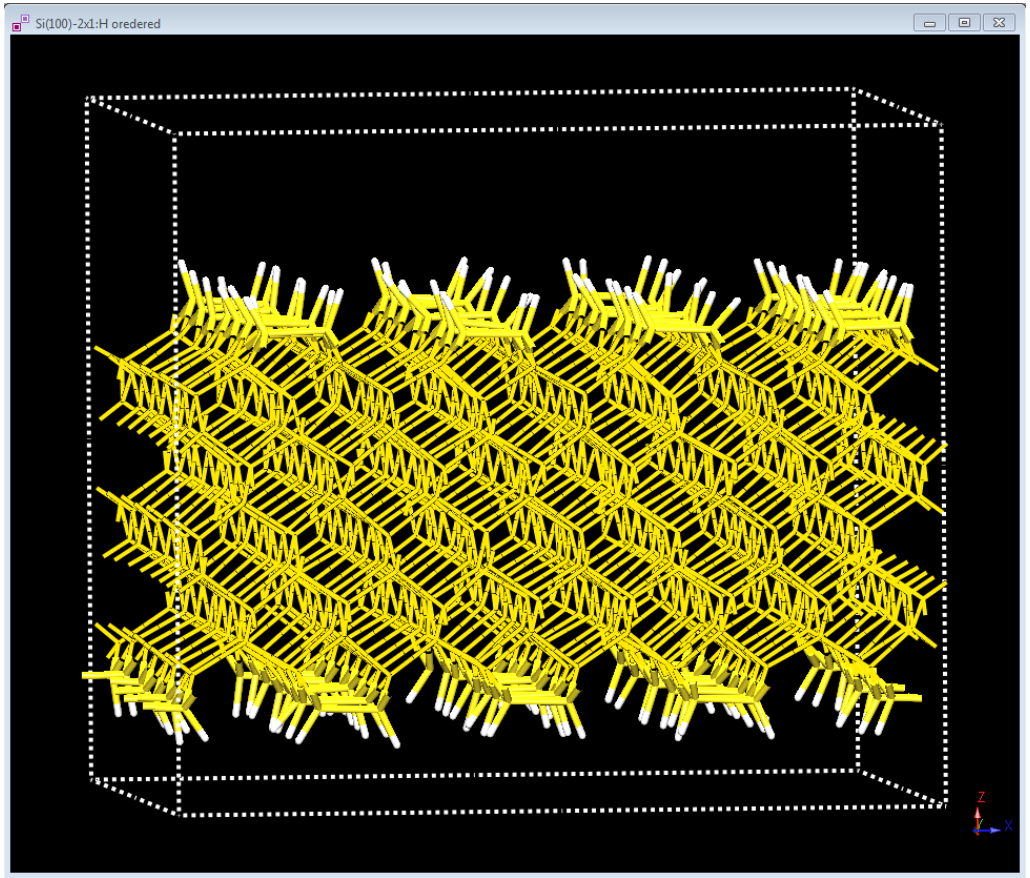
Tersoff Potential Validation

- Reproducing structural characteristics:
  - Si(100)–2x1 reconstruction
  - Si(100)-2x1 reconstructed, H terminated
    - Si-Si : 2.4 Å
    - Si-H : 1.521 Å
    - Si-Si-H : 111.9 deg



Ohira et al, *Phys. Rev. B*, 52, 8283, 1995
Ohira et al, *Surface Science,* 458, 216–228, 2000

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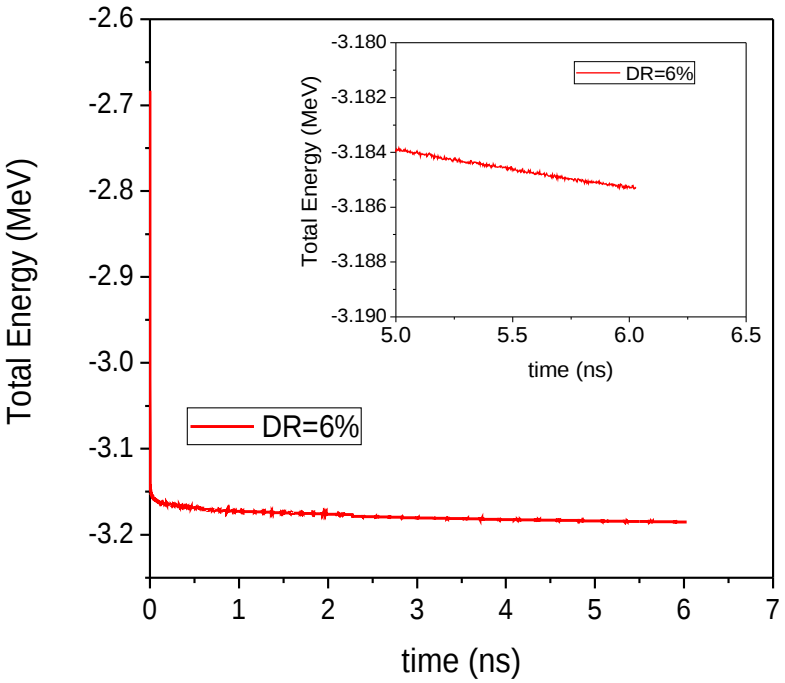
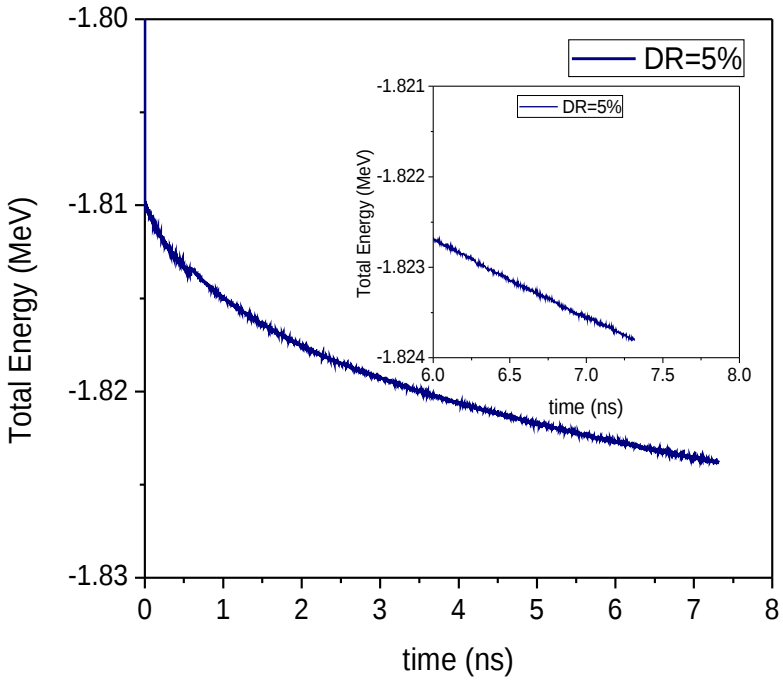
LAMMPS MD Results:

- **Convergence of total energy:**





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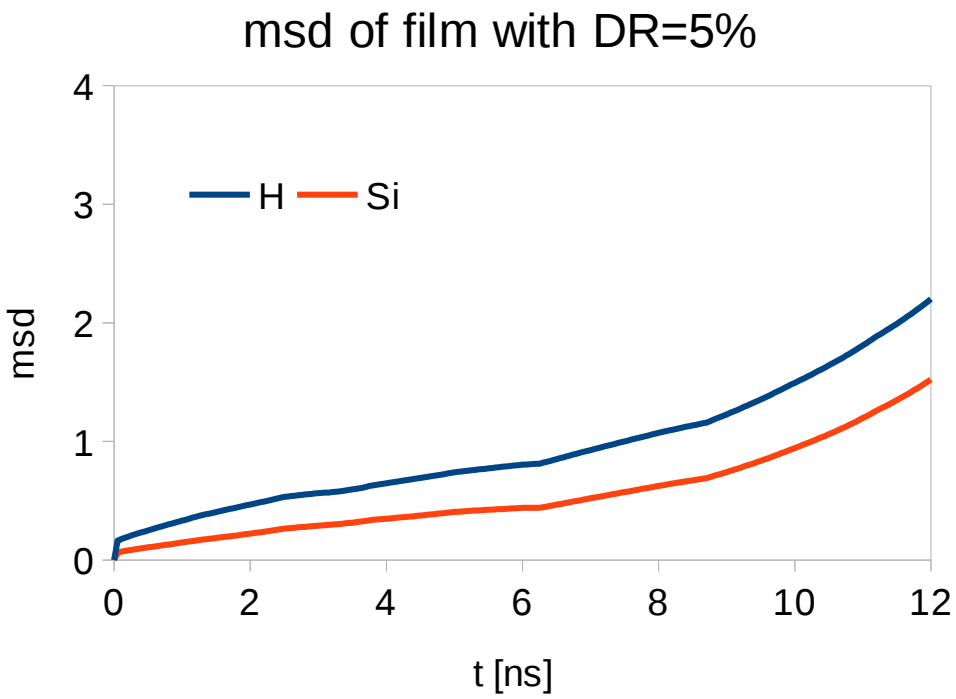
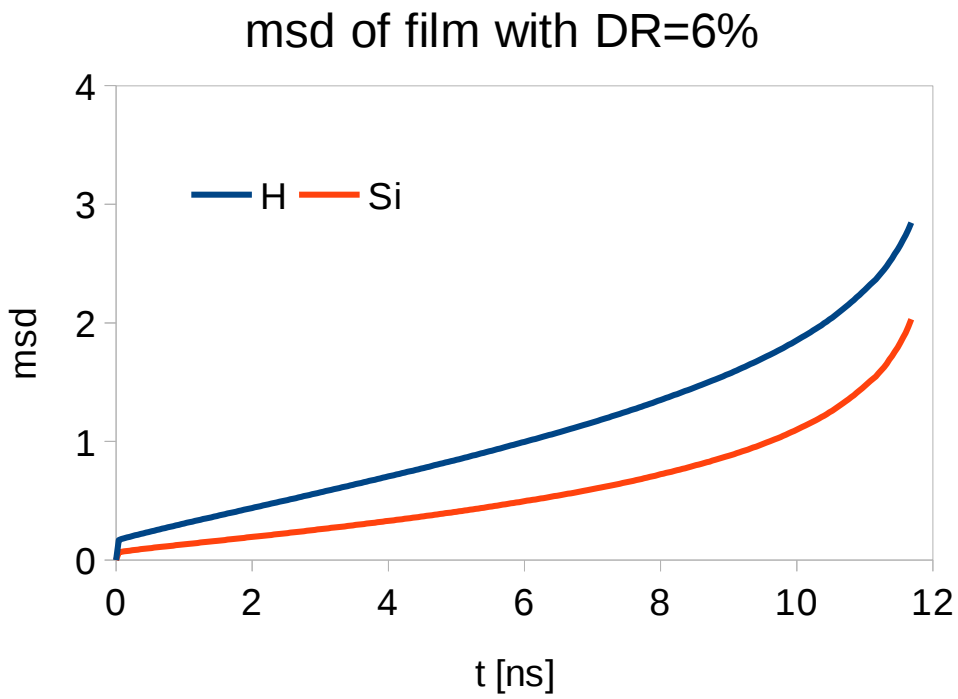
LAMMPS MD Results:

- **Diffusion and Mean Square Displacement:**





DR = 5 %

DR = 6 %

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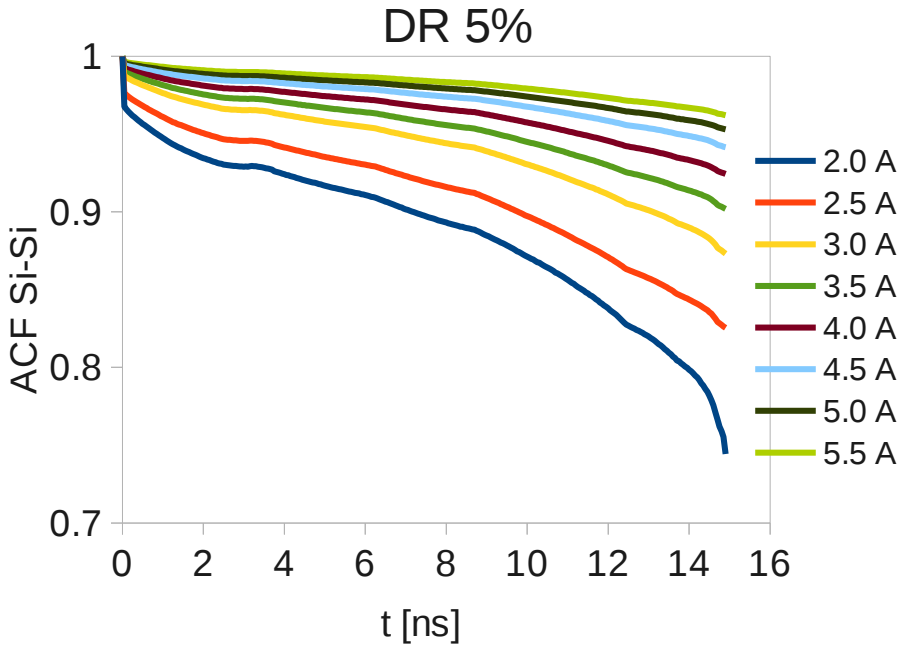
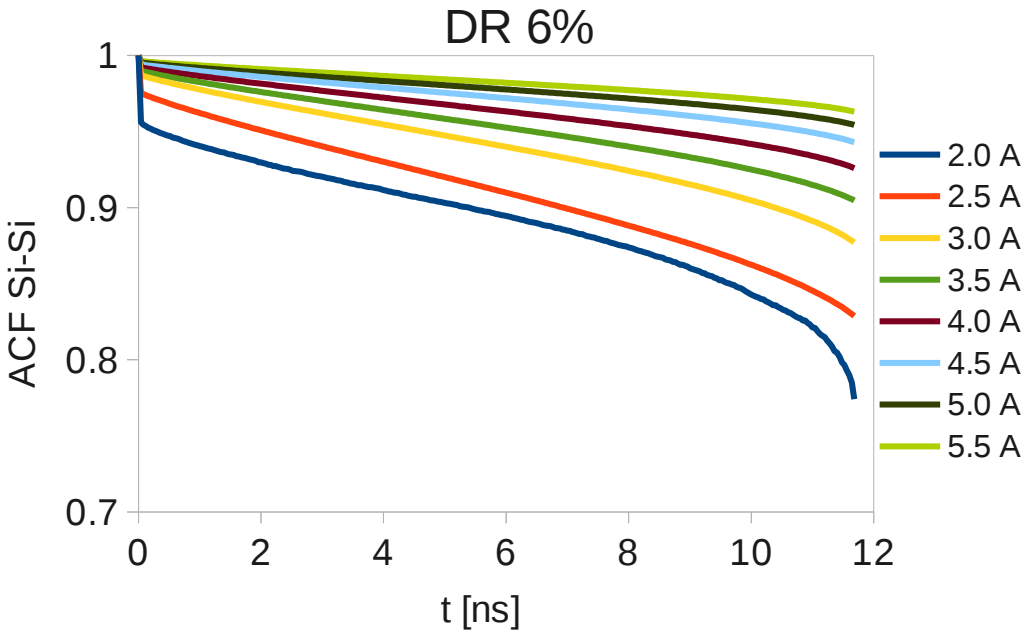
LAMMPS MD Results:

- **Autocorrelation functions:**





DR = 5 %

DR = 6 %

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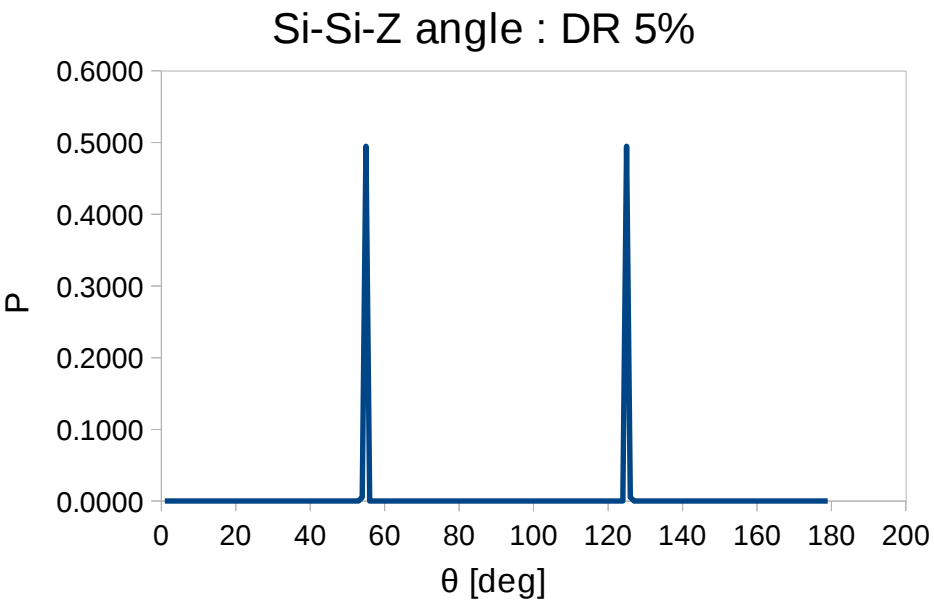
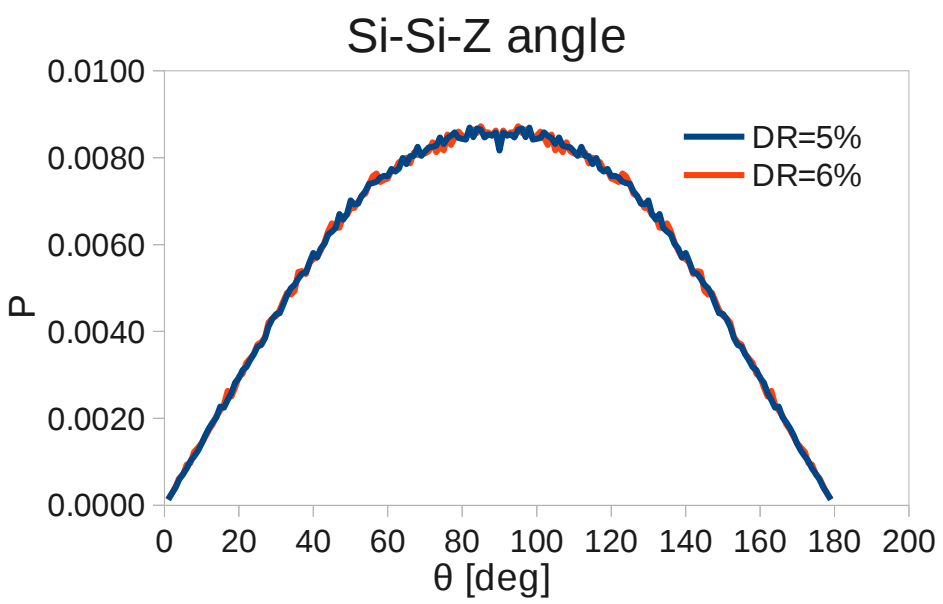
LAMMPS MD Results:

- **Bond Angle Distribution:**





After MC

After MD

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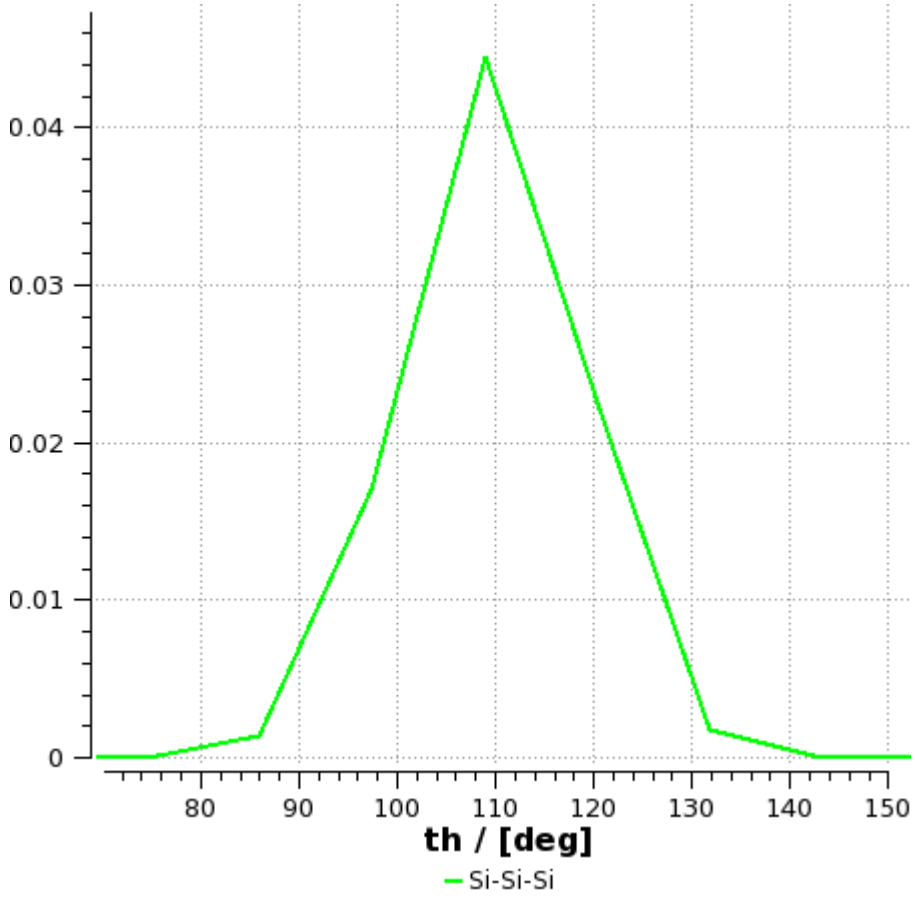
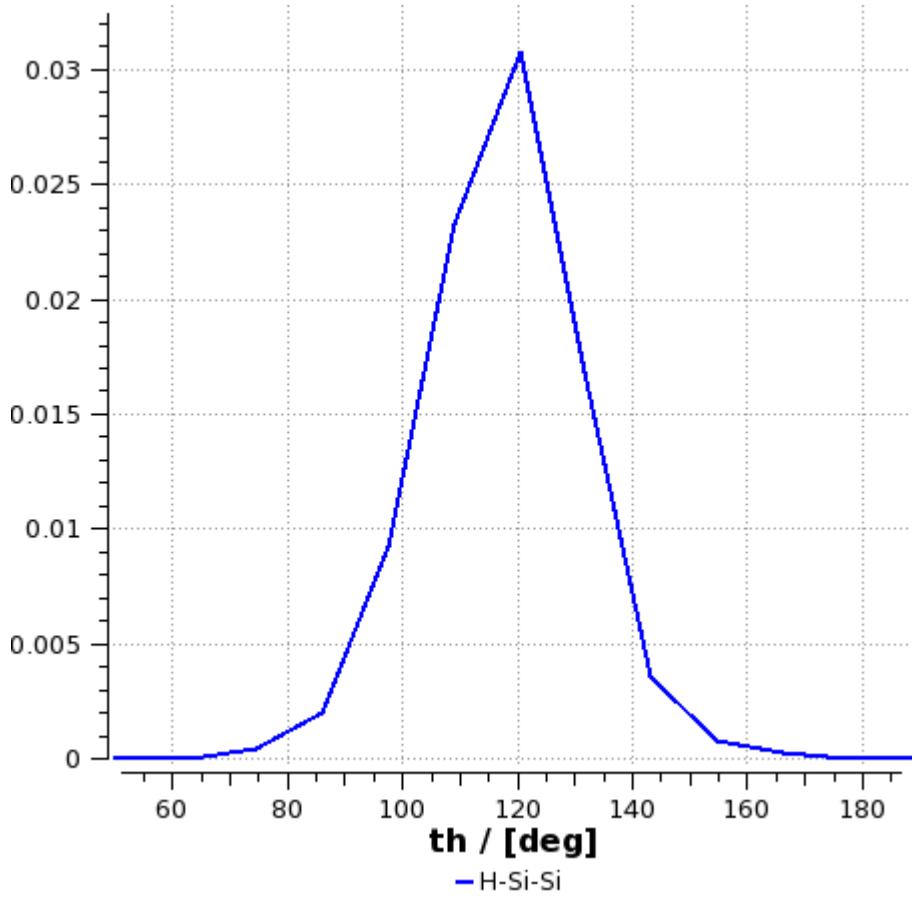
LAMMPS MD Results:

- **Bond Angle Distribution:**





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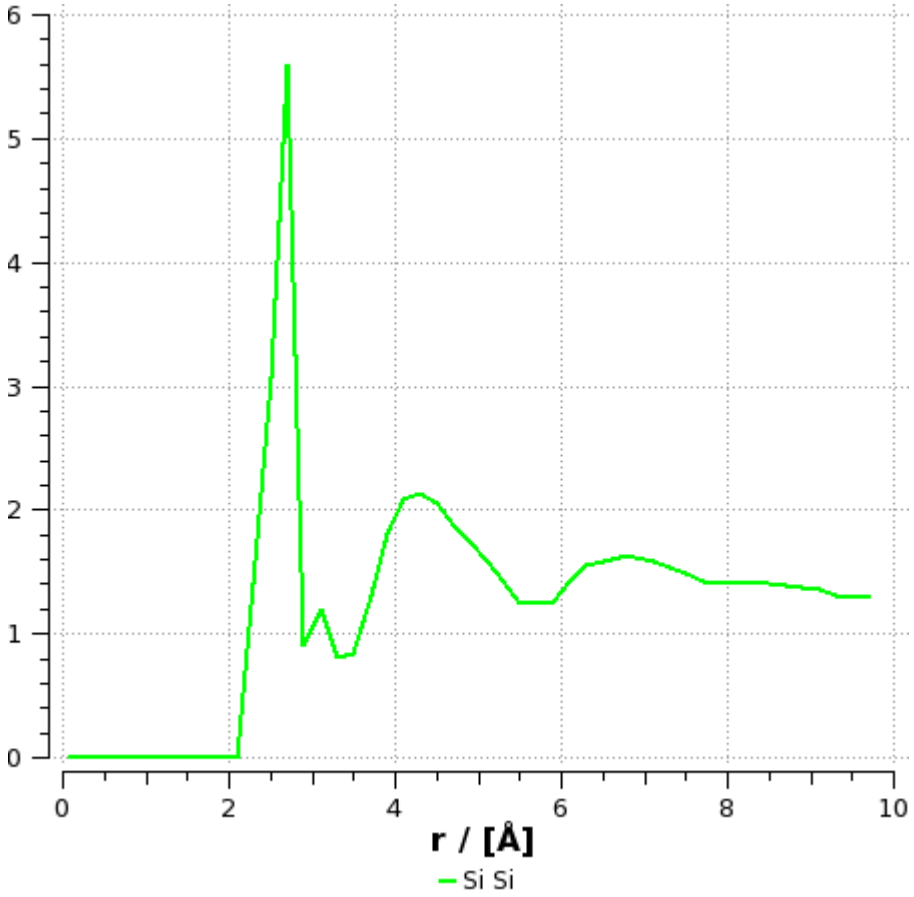
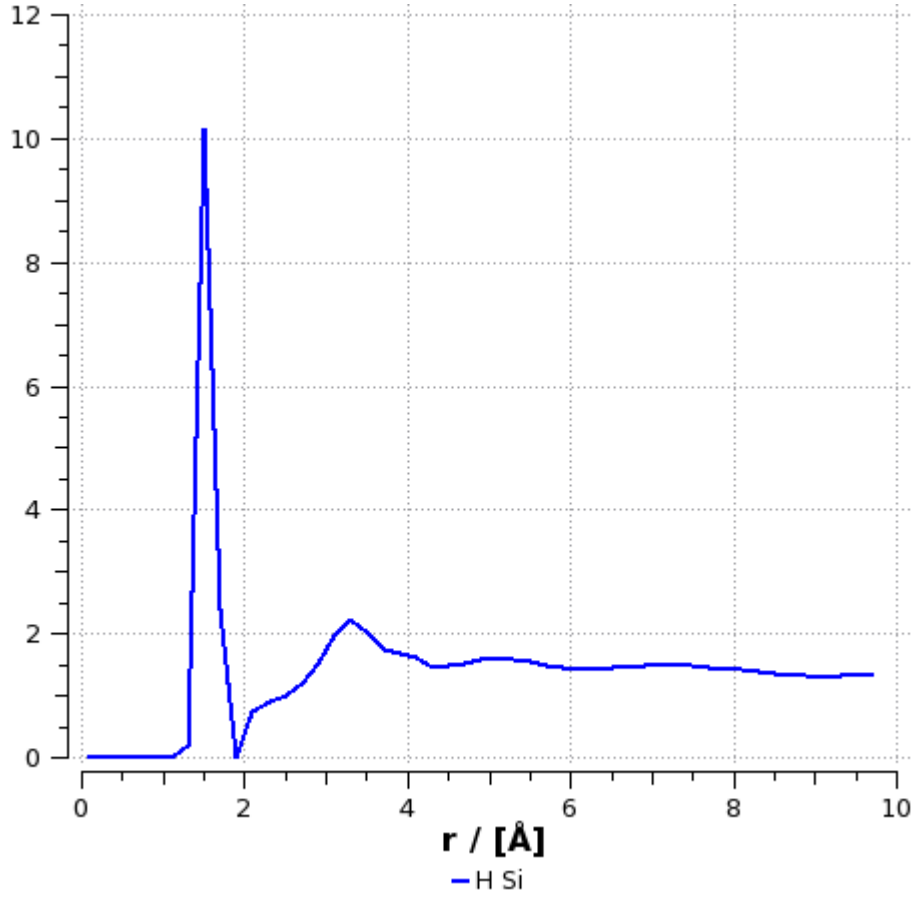
LAMMPS MD Results:

- **Pair Correlation functions:**





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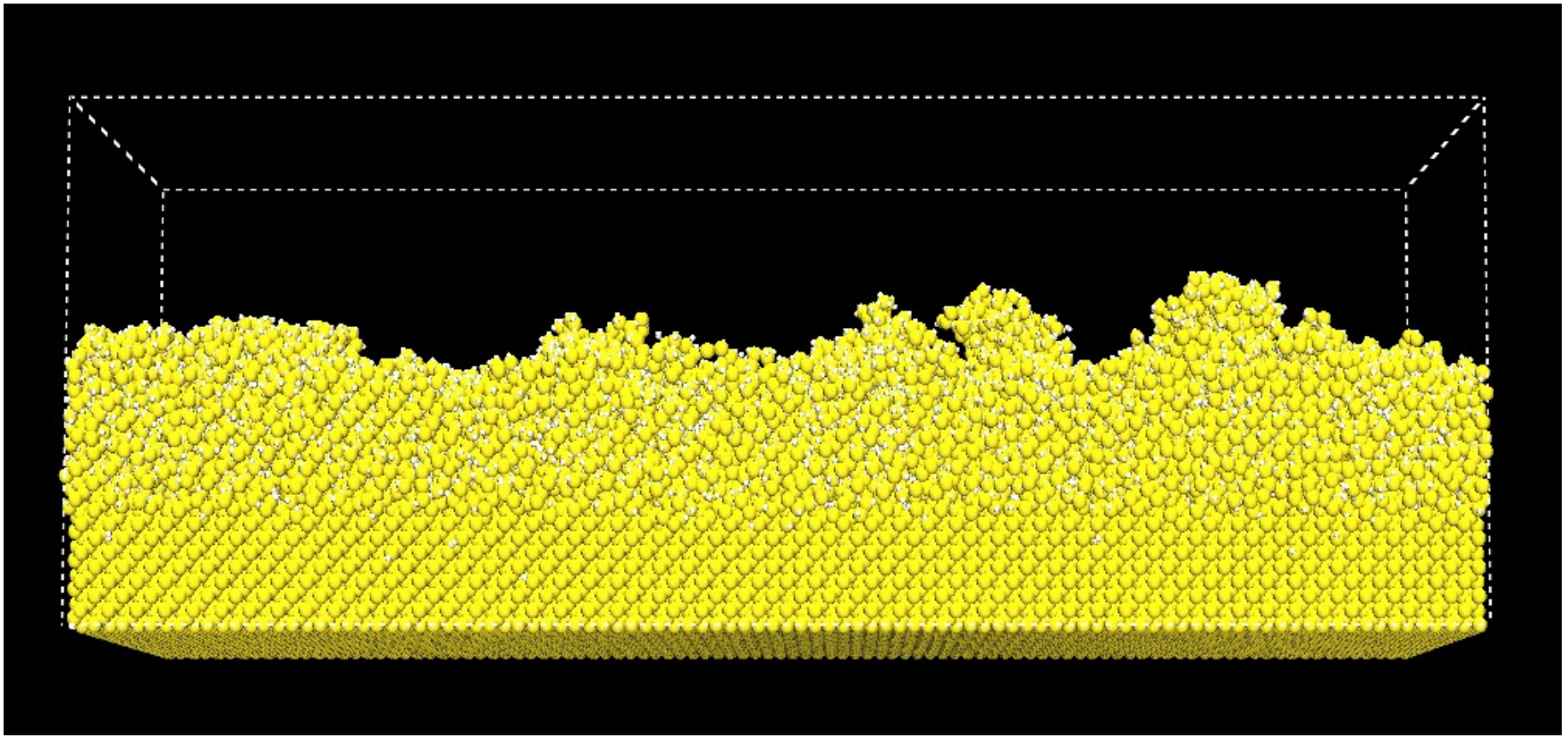
LAMMPS MD Results:

- **Structure on substrate visualized in MAPS after MD relaxation**



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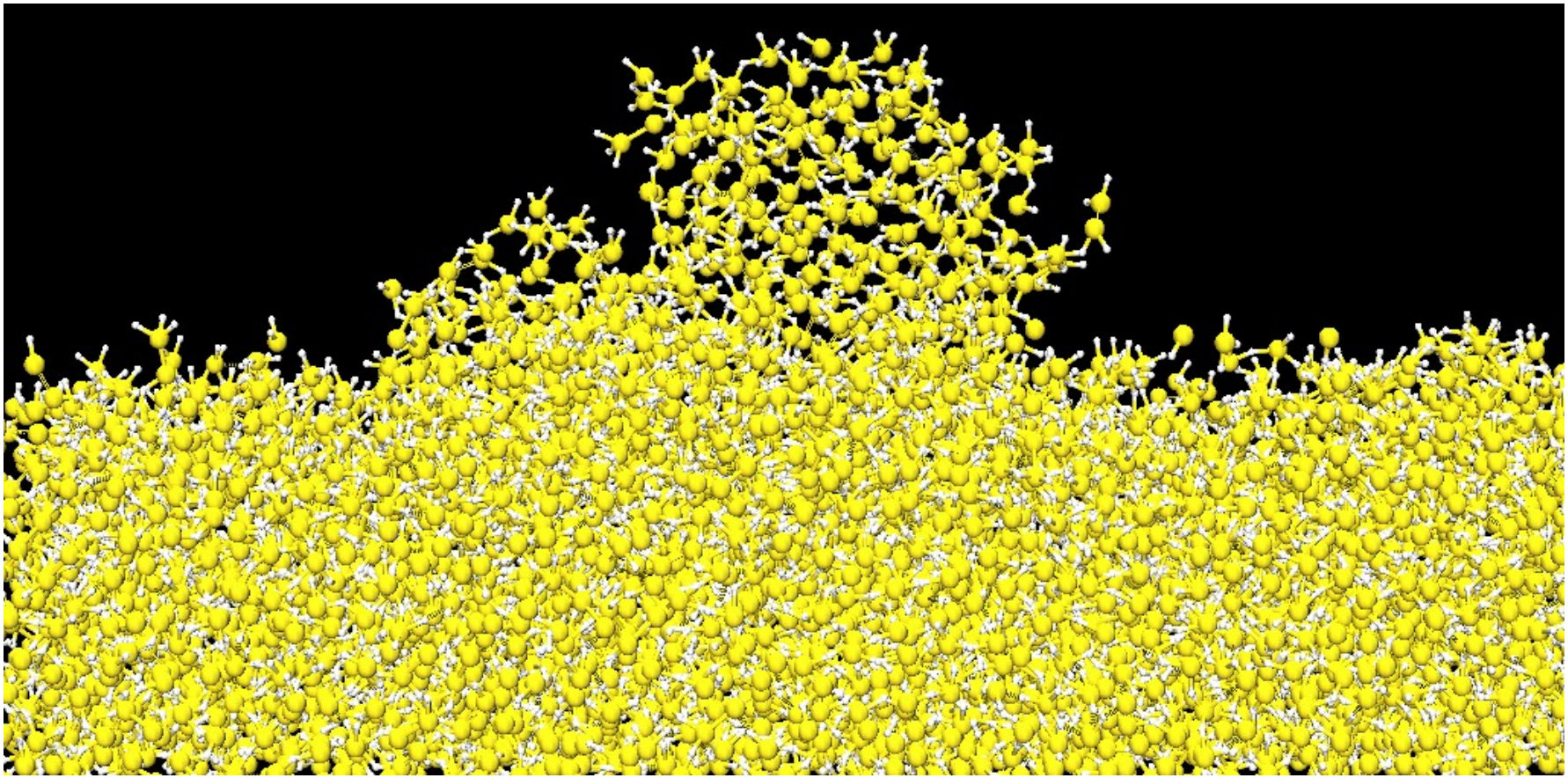
LAMMPS MD Results:

- **Local Growth Zone in some detail**



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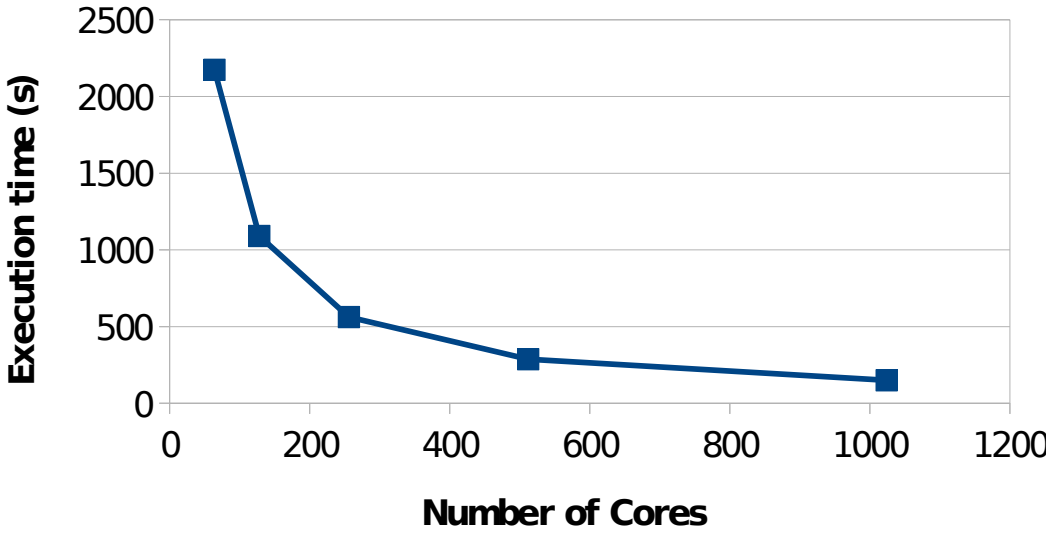
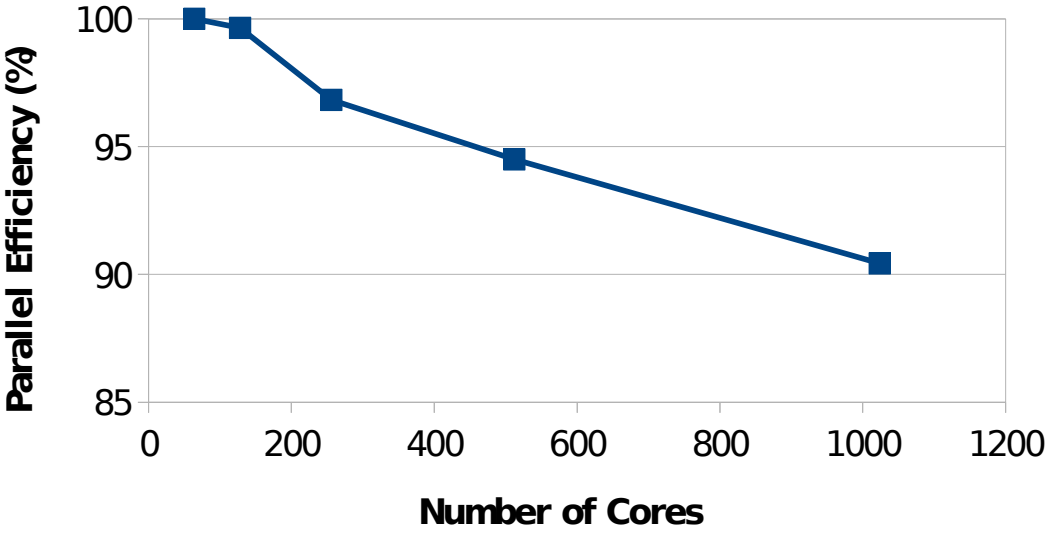
LAMMPS MD Performance with modified Tersoff potential:

- Execution time over 10000 MD steps
- System size 965902 atoms, 80000 fixed NVT with PBC in x and y





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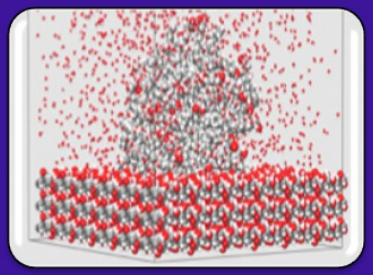
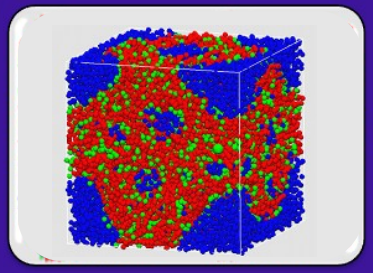
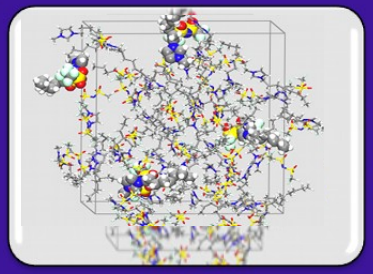
Classical Engines & Tools in MAPS



LAMMPS: A comprehensive package for molecular dynamics and mechanics simulations of periodic and non periodic systems



LAMMPS-DPD: Perform Dissipative Particle Dynamics simulations to study the mesoscopic behavior of fluids and related materials



NAMD: A molecular dynamics and mechanics simulations package for studying dynamic phenomena and bulk properties of large molecular systems

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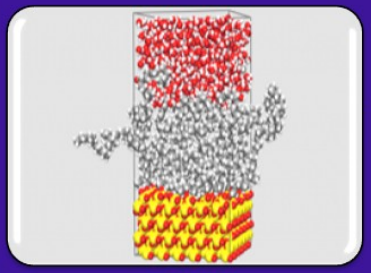
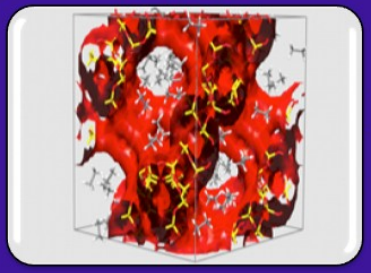
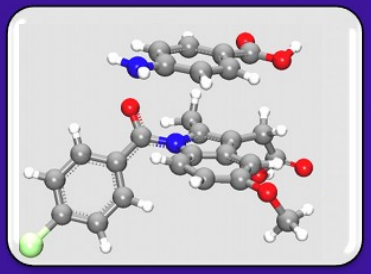
Monte Carlo based Tools



Amorphous Builder: State-of-the-art Monte Carlo based technology for building realistic models of amorphous and nano-structured materials



Towhee: A comprehensive package for Monte Carlo simulations of periodic materials in various ensembles



FHMixing: A Monte Carlo based simulation engine for the rapid estimation of thermodynamic properties of binary mixtures

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Scienomics LAMMPS additions

- Tersoff with repulsive three body interactions (tersoff/rep) – will be committed soon
- Bond angle: fourier, fourier/simple, quartic
- Dihedral: quadratic, nharmonic
- Improper: fourier

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Conclusions

- **Silicon films growth by PECVD modeled using KMC combined with MD**
- **With KMC:**
  - overcome the problem of multiple time scales of the reactions involved in the process
  - good qualitative prediction of the deposition rate for a range of conditions
  - good qualitative prediction of the final composition in H for a range of conditions
  - Film thickness of several 10 nm simulated
- **With the MD simulations we target:**
  - Relaxation of the films produced from KMC
  - Gradual relaxation of the film as it is developed fro KMC
  - Study the molecular mechanisms relevant to properties such as crystallinity and surface roughness

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Thank you for your attention

Contact:
Andreas.Bick@scienomics.com
Visit: www.scienomics.com

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