MedeA Deposition

Atomistic-Scale Simulations of Deposition, Growth, Oxidation, and Etching at your Fingertips

At-a-Glance

Interactions between particles and surfaces control many important processes including deposition, oxidation, growth, surface modification, bombardment, sputtering, and etching. The *MedeA*®[1] *Deposition* module facilitates the simulations of automated, continuous impact of pre-defined particles on to a surface and enables you to examine the dynamical processes and mechanisms that govern particle-surface reactions and interactions.

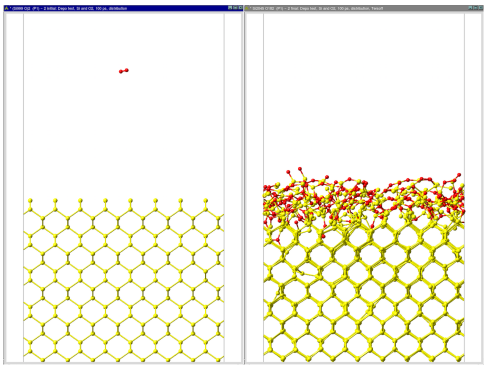
Key Benefits

- Deposition of any amount of various particle types such as atoms, cluster, and molecules
- Impact the surface with user-defined particle velocities or energies, angles, and frequencies
- Automated analysis of results such as particle distribution plots

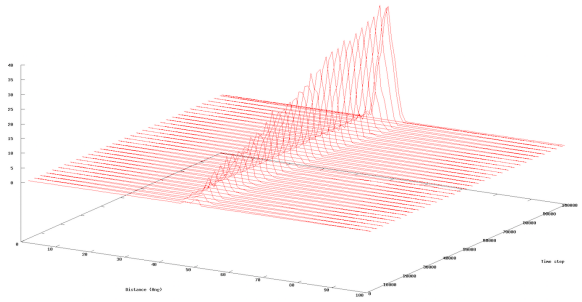
[1] MedeA and Materials Design are registered trademarks of Materials Design, Inc.

Computational Characteristics

- Users define impact region, impact velocity/energy, impact angle, impact frequency, and total number of deposits per deposition particle type



- *MedeA Deposition* uses the LAMMPS classical molecular dynamics engine for efficient performance on computers from scalar workstations to massively parallel supercomputers
- Temperature control of the substrate with the Langevin thermostat
- Creates distribution plots automatically per deposition particle type for analyses of penetration depth, reaction range, growth thickness, etc.



- Works with reactive forcefields such as ReaxFF, COMB3, Tersoff, and EAM, as well as non-reactive valence forcefields such as PCFF+

Required Modules

- *MedeA Environment*
- *MedeA Deposition*

Recommended Modules

- *MedeA ReaxFF*, *MedeA COMB3*, and *MedeA EAM*

Find Out More

Contact Materials Design to see how *MedeA Deposition* can be employed in the following tutorials:

- Deposition of O_2 on Si Surface with reactive forcefields

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