

MedeA Deposition

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

At-a-Glance

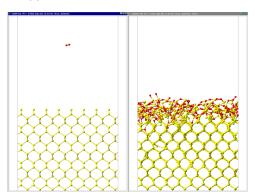
Interactions between particles and surfaces control many important processes including deposition, including Micro-cold spray, or oxidation, growth, surface modification, bombardment, sputtering, and etching. The *MedeA Deposition* module facilitates the simulations of automated, continuous impact of 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
- Study the effects of deposition parameters on surface morphology and atomic distribution
- Automated analysis of results such as particle distribution plots

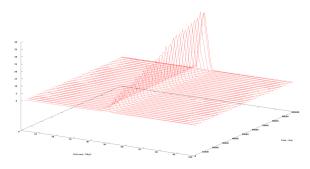
Computational Characteristics

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



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

Required Modules

- MedeA Environment
- MedeA Deposition

Recommended Modules

 MedeA MLP, 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 O₂ on Si Surface with reactive forcefields









