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

Contents

1 Introduction

Interactions between particles and surfaces control many important processes including deposition, oxidation, growth, surface modification, bombardment, sputtering, and etching. The *MedeA Deposition* module facilitates the simulations of the automated, continuous impact of pre-defined particles onto 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, clusters, and molecules

- Impact the surface with user-defined particle velocities or energies, angles, and frequencies

- Automated analysis of results such as particle distribution plots

2 Computational Characteristics

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

- *MedeA Deposition* uses the LAMMPS classical molecular dynamics engine (MedeA LAMMPS) for efficient performance on computers ranging 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+*

Hint: The *MedeA Deposition* module works with the classical molecular dynamics engine LAMMPS. Ab initio molecular dynamics simulations are currently not supported. For more information on LAMMPS within *MedeA*, see section MedeA LAMMPS.

DOCUMENTATION

3 Input Structure Preparation

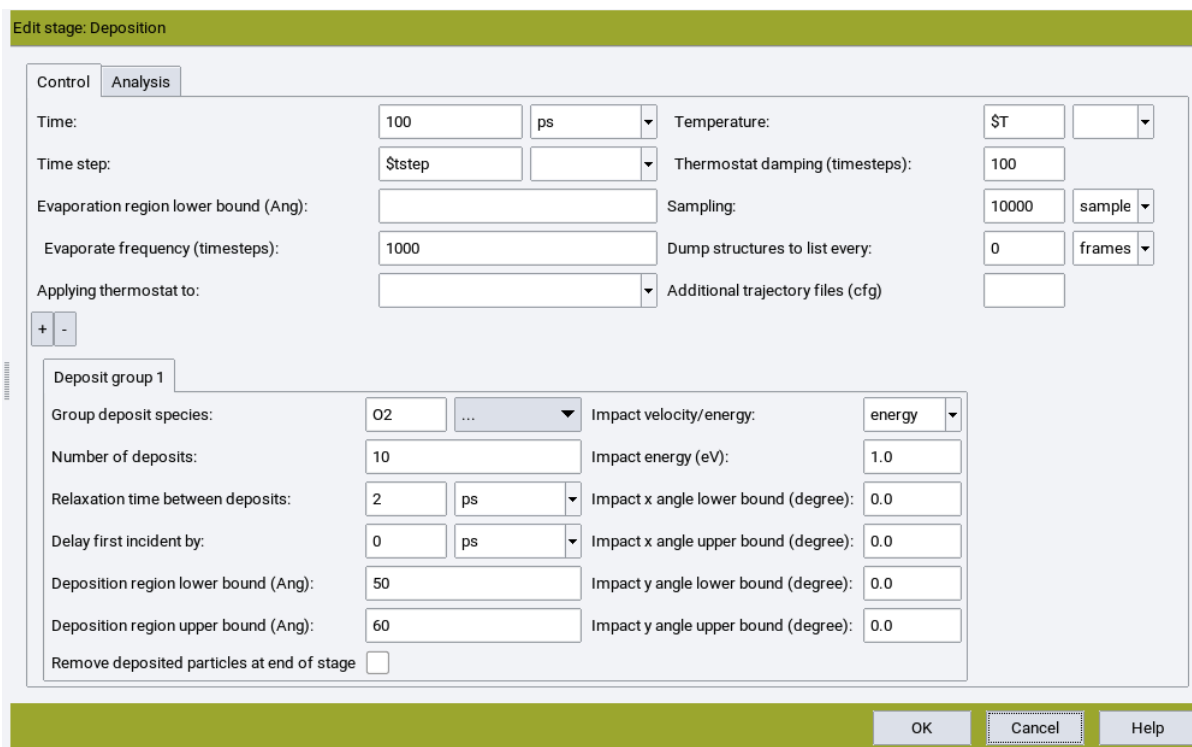The *MedeA Deposition* module requires the following input:

1. A surface with a plane normal to the Z direction

2. Enough vacuum space (usually more than 30 Å but dependent upon your system) so that deposited atoms and molecules can accumulate on the surface

3. One or more subsets each containing one atom, fragment, or molecule in the vacuum space

> **Warning:** Caution should be exercised if wanting to add an **NVT** or **NPT** stage for equilibration prior to the deposition stage. It is possible for the molecule used for deposition to dissociate, react, or otherwise have significant changes to the internal geometry of the molecule during the NVT stage. The **Deposition** stage uses the configuration of the molecule chosen for deposition that is available immediately prior to to the **Deposition** stage and not the configuration that is given in the initial structure. A safer alternative is to use a separate Flowchart to equilibrate the initial structure and then insert the species used for deposition. This equilibrated structure with the deposition species added can then be used in the Flowchart involving the **Deposition** stage ensuring that the desired template geometry for the deposition species is used.

4 The *MedeA Deposition* Module

The *MedeA Deposition* module can be accessed within any *MedeA LAMMPS* Flowchart by adding a **Deposition** stage. One or more pre-defined subset(s) of atoms or molecules are inserted to the vacuum region and impact the surface with user-defined velocities, angles, etc. Automated analysis of simulation results completes the workflow.

This is a screenshot of the **Deposition** stage GUI:

Input parameters are:

- *Time*: Duration of the simulation run. The appropriate value for this parameter depends on the *Number of deposits*, *N*, and *Relaxation time between deposits*, *t*. Usually $T = N * t + C$ where *C* is an

additional several ps to allow all deposits to equilibrate.

- *Time step*: Time step size employed in solving the equations of motion in an NVE ensemble.

- *Evaporation region lower bound (Ang)*: Can be added to remove atoms, molecules, and/or fragments leaving the surface so they do not accumulate at the upper boundary or re-enter the periodic boundary condition and deposit on the bottom surface. Usually, 5–10 Å smaller than box size.

    - *Evaporation frequency (timesteps)*: Detect if there are any atoms in the evaporation region every this many steps. Usually, 100–1000 is a good number. The default is `1000` steps. Not used if the above option is blank.

- *Applying thermostat to*: Add Langevin thermostat to a pre-defined subset of atoms. Usually, the subset region comprises several layers to several 10s of layers of atoms in the middle section of the slab. This can regulate overall system temperature but does not significantly affect dynamics at the surface.

    - *Temperature*: Langevin thermostat temperature. Not used if the above option is blank.

    - *Thermostat damping (timesteps)*: Langevin thermostat strength. A smaller value means a more aggressive thermostat. Usually, the default of `100` time steps is sufficient.

- *Sampling*: Number of samples employed in each average. This parameter does not affect dynamics.

- *Dump structures to list every*: Together with *Time*, determines the number of trajectory frames saved to a structure list during the molecular dynamics calculation. This parameter does not affect dynamics.

- *Additional trajectory files (cfg)*: Write additional trajectory files in the cfg format used by the *AtomEye* visualization software.

The bottom panel controls each of the deposit groups. Use the `+` and `-` buttons to add or remove a deposit group.

- *Group deposit species*: Name of the pre-defined depositing subset.

- *Number of deposits*: Deposit this many atoms or molecules onto the surface for the entire simulation.

- *Relaxation time between deposits*: Time interval between deposition events.

- *Delay first incident by*: Can be used to delay deposition events so if you have multiple depositing groups you can alternate deposition events.

- *Deposition region lower bound (Ang)*: Lower bound of the region to insert new depositing species.

- *Deposition region upper bound (Ang)*: Upper bound of the region to insert new depositing species. New depositing species are inserted randomly within the lower and upper bounds.

- *Impact velocity/energy*: A drop-down menu to choose between impact energy (eV) or impact velocity (m/s).

Note: If impact energy is selected, the energy value is internally converted to a velocity value based on the composition of the deposition species. The impact velocity that is specified, or computed, is then used to sample a uniform distribution of impact velocities in a range $\pm$ 10% of the user-provided value. Thus, the deposited species are initialized with slightly different initial velocities.

- *Impact x angle lower bound (degree)*: Add -X velocity to depositing species.

- *Impact y angle upper bound (degree)*: Add +X velocity to depositing species.

- *Impact x angle lower bound (degree)*: Add -Y velocity to depositing species.

- *Impact y angle upper bound (degree)*: Add +Y velocity to depositing species.

Note: The X/Y angles and lower/upper bounds allow angled deposition events.

- *Remove deposited particles at end of stage*: Useful if you want to more closely examine the surface without depositing species.

5 Distribution Analysis

Distribution analysis is available in the second tab of the **Deposition** stage:
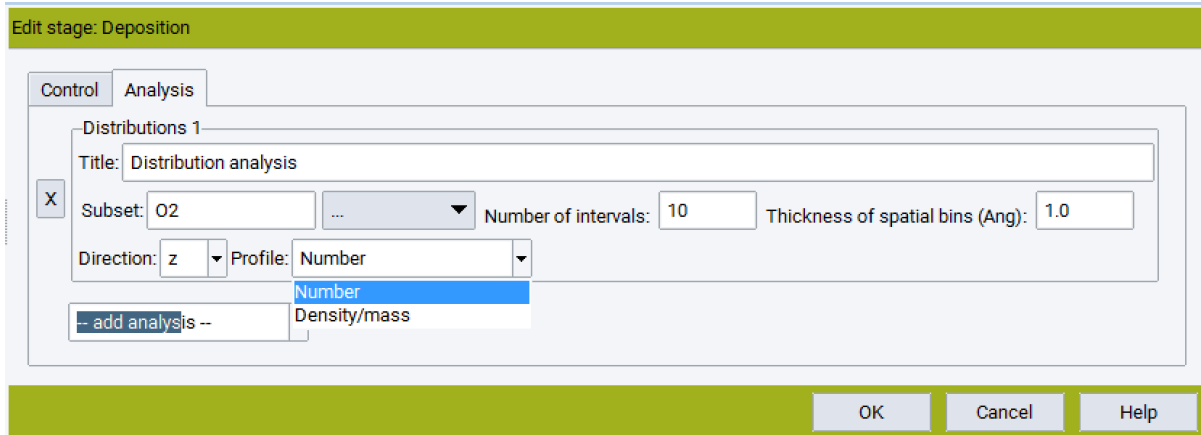
Input parameters are:

- *Title*: Title of the distribution analysis output.
- *Subset*: Name of the pre-defined depositing subset to be analyzed; choose from the drop-down menu.
- *Number of intervals*: Number of analyses to perform throughout the simulation.
- *Thickness of spatial bins (Ang)*: Size of the bins used for histogramming results.
- *Direction*: Plot distribution along this direction. The default is z .
- *Profile*: Number or Density/mass for number or mass density, respectively.

Example output:
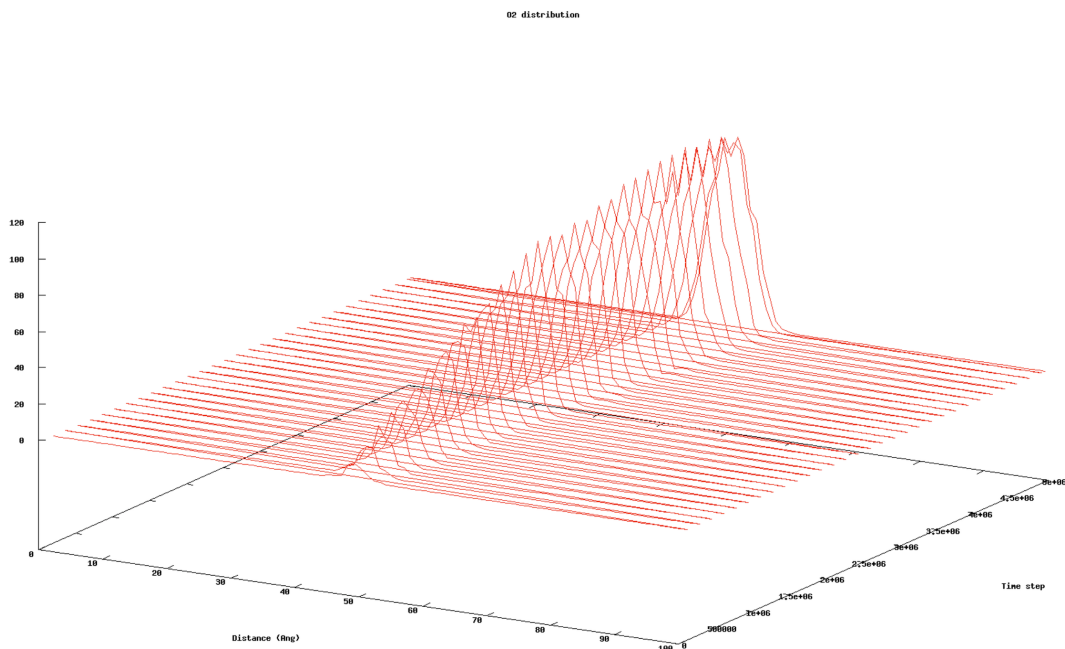
- Vertical axis: Number of deposited species.
- Horizontal axis: Distance (or height) along the defined direction.
- Depth axis: Simulation time step.